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Modeling of Simulated Photchemical Smog with Kinetic Mechanisms. Volume 2. CHEMK: A Computer Modeling Scheme for Chemical Kinetics

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Volume 2. CHEMK: A Computer Modeling Scheme for Chemical Kinetics

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MODELING OF SIMULATED PHOTOCHEMICAL SMOG WITH KINETIC MECHANISMS
Volume 2. CHEMK: A Computer Modeling Scheme for Chemical Kinetics

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ABSTRACT

Mechanisms that describe the formation of photochemical smog are developed using a computer modeling technique directed toward the simulation of data collected in two smog chambers: an indoor chamber and a dual outdoor chamber. The results of simulating 164 different experiemnts are presented in Vol. I. Individual compounds for which specific experiments were simulated and mechanisms developed include the following: formaldehyde, acetaldehyde, ethylene, propylene, butane, and toluene. Experiments in both chambers were simulated for all these compounds. The mechanisms reported describe the decay of the precursor organic compound, formation and decay of secondary organics, conversion of nitrogen oxides, formation of nitrates, and the appearance and decay of ozone. Special emphasis is given to the chemistry of toluene. Also included is a study of a generalized smog-based or carbon-bond mechanism developed in a previous study. Vol. II contains the user's manual and coding for a chemical kinetics computer program, CHEMK.

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SECTION 1

INTRODUCTION

Calculation of the time-dependent concentration profiles of a number of reacting species in a complex reaction mechanism is central to the science of chemical kinetics. Such calculations allow the validation of kinetic schemes and reaction rate constants through the comparison of predicted concentrations with experimental data. The need to rely on approximation methods such as steady-state assumptions, quantum yields, and a "rate-determining step" in making these calculations adds uncertainty to predicted concentrations and could possibly conceal inaccuracies in the kinetic mechanism if the experimental data were highly scattered. These approximation methods are also time-consuming in that the user must formulate them and evaluate their impact on the predictions.

Work by Whitten (1974) and Overton (1976) led to the development of fast and efficient computer programs that make complex calculations commonplace. These computer programs integrate the system of ordinary differential equations (ODEs) associated with a kinetic mechanism, given a set of initial conditions. The method used to integrate the system of ODEs was developed by Gear (1971) and modified by Hindmarsh (1974). Initial work by Whitten (1974) led to the development of a computer program that could handle 50 chemical species and 200 chemical reactions. That program, CHEMK, used the modified Gear routines documented by Hindmarsh (1974).

Since that time Spellmann and Hindmarsh (1975) have modified the Gear routines to handle sparse matrices. The Jacobian, or the matrix of partial differential equations, associated with a given chemical kinetic mechanism is usually sparse, meaning that it contains more zero elements than non-zero elements. Thus, the use of a routine designed specifically for sparse matrices would increase the efficiency of the computer program CHEMK in terms of central processing (CP) time. The work of Spellman and Hindmarsh

and our experience with the limitations of the first versions of CHEMK led us to modify CHEMK.

In this report, we present a new version of CHEMK that can handle chemical kinetic mechanisms containing up to 89 species and up to 200 reactions. The new version can also handle photolysis rate constants and temperatures that vary with time, and reaction schemes with stoichiometric coefficients. The Gear routine used is that of Spellmann and Hindmarsh referred to above.

The version of CHEMK documented in this report requires approximately 44000 decimal words to load on a Control Data Corporation (CDC) 7600 computer. The efficiency of the new program has been increased about a factor of 3 from the original versions of CHEMK. Rather than present a detailed description of the program and its various routines, the emphasis in this report has been placed on providing a description of program inputs and options available to the user. A complete program listing is provided in Appendix A. Appendices B and C give the input data for an example run in the CHEMK and the EPA format, respectively. Appendix D gives the output of that example run in EPA format, and Appendix E provides an example of variable photolysis and print options.

SECTION 2

CHEMK INPUT

A brief description of each data input card and its argument list is given below. Both initial program specification and modified operation are treated in this presentation. The data input flow is illustrated schematically in Figure 1.

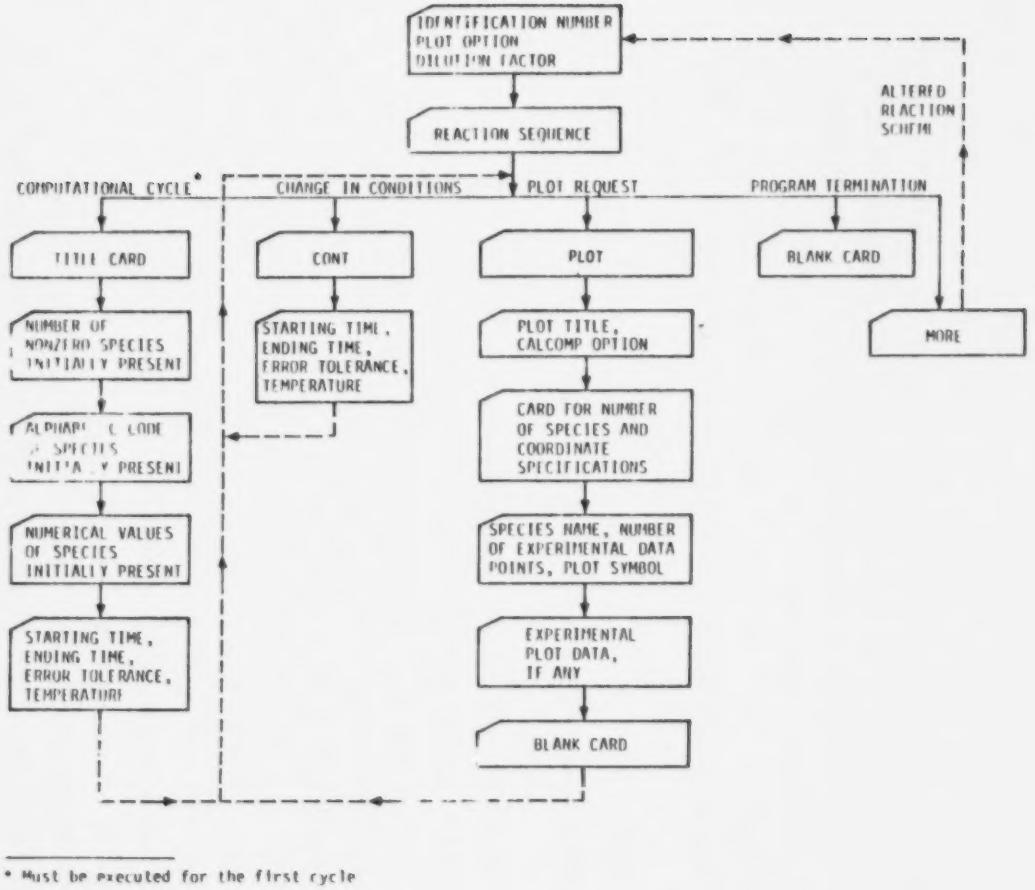
BASIC INPUT FOR A NEW PROBLEM

General Data Card

The arguments that can be entered on this card are:

- The last number of the reaction sequence.
- Choice of reaction format.
- Print option to print only instantaneous concentrations at specified intervals.
- Dilution factor.
- Number of time intervals in which the photolysis rate constants are changing.
- The time interval of each photolysis number.
- The number of photolysis reactions.
- The number of temperature values.
- The time interval of each temperature value.
- Option to plot the photolysis values as a function of time.

The last number of the reaction sequence should correspond to the number on the last card in the reaction scheme, even though it is not the highest reaction number. The next parameter (choice of reaction format) is to enable users of EPASIM (Overton, 1976) and users of the first versions of



* Must be executed for the first cycle

Figure 1. Data input flow chart

CHEMK to use the current version of CHEMK. A more detailed discussion of this option is presented in the section on kinetic mechanism cards.

An option has been added to the CHEMK program that will control the printing of the species' net rates of formation and the net rates of reaction. When this option is not used, only species concentrations are printed at specified time intervals.

To activate this option so that species net rates of formation and net rates of reaction will be printed at the same specified time intervals, the user enters any alphanumeric character anywhere in columns 11 through 14 of the General Data Card.

The dilution factor represents a constant dilution rate for every species such that:

$$\frac{dC_i}{dt} = -DC_i \qquad (1)$$

where

C_i = concentration of species i
D = dilution factor.

In many experiments all species are being diluted by a common first-order factor. If this factor is entered in the third field of the General Data Card (the one that identifies the last reaction and on all subsequent appearances of such a card), then this option will be activated. If one species (e.g., O_2) is part of the dilution gas, a first order "flow out" (e.g., O_2, the only reactant with no products) reaction with a negative rate constant equal to the dilution factor will cancel the dilution for such a species.

The next three parameters (number of time intervals in which the photolysis rate constants are changing, the time interval of each photolysis number, and number of photolysis reactions) are used to input the conditions of the time-varying photolysis rate constants. If a blank or zero is entered for the number of time intervals, then the time interval and number of photolysis reactions should not be entered. If the number of time intervals is nonzero ther the first card after the General Data Card should contain the vector of reaction numbers that identify the reactions with varying photolysis rate constants. Up to seven numbers may be placed on each card.

The next card(s) will contain the initial photolysis value and the values at the end of each time interval. If, for example, the user inputs 5 as the number of time intervals and 60 (minutes) as the time interval, then six photolysis values should be entered on the card (one for the initial value and one for every 60 minutes thereafter). Up to seven photolysis values may be entered on one card. The total time in which the photolysis rate constants are changing in the above example is 300 minutes. If the simulation is carried for a longer period of time (e.g., 600 minutes) then all photolysis rate constants are set to zero after 300 minutes. The maximum number of time intervals is 97 for each simulation. If more values are needed the MORE option may be used (see section on MORE option).

If the number of temperature values is nonzero, the next set of cards is the vector of temperature values (initial plus the end of each time interval specified on the General Data Card). The format for the temperature values is similar to that for the photolysis values. All temperature values must be in units of degrees Kelvin (K). All activation energies entered on each reaction card must also be in units of degrees Kelvin. The temperature at each specified printout time is printed with the rest of the species under the column TEMP.

If the user wishes to obtain a plot of the photolysis values as a function of time, then a nonzero value is declared in columns 56 to 60. A line printer plot is produced at the end of the species concentration versus time profiles. This option should be activated only when the plot option is declared.

2. Kinetic Mechanism Cards

Each chemical reaction in the mechanism must be entered individually. Entry requires (1) that the reaction be numbered, (2) that its components be specified in alphanumeric form, and (3) that the rate constant at 298K be specified. If the reaction is temperature-dependent, then the activation energy (in degrees Kelvin) can also be specified. A maximum of 200 reactions is allowed by the program.

The user has a choice of two different input formats for the reactions. To accommodate users of EPASIM (Overton, 1976) CHEMK allows nonunity stoichiometric coefficients for the products of the reactions. The reaction input format described in EPASIM and summarized in Table 1 is available for users of EPASIM and the current version of CHEMK. A maximum of three reactants and three products (with stoichiometric coefficients) are allowed under the EPASIM format. To use the EPASIM format, the user must enter a nonzero value in the second field of the General Data Card (see preceding subsection).

Reaction identification numbers are not used under the EPASIM format as described by Overton (1976). Therefore, we introduced this parameter in columns 17, 18, and 24 of the reaction card. The first field represents the reaction number from 1 through 99. If the user has more than 99 reactions, a modulus factor must be specified in column 24 to convert the reaction number to a number greater than 100. For example, a reaction identification number of 13 is given on the reaction card in columns 17 and 18 while column 24 is left blank. A reaction identification number of 123 is given on the

reaction card first by input of 23 in columns 17 and 18 and 1 in column 24. For reaction 200, columns 17 and 18 are left blank (representing zero) and a 2 is entered in column 24.

For users of earlier versions of CHEMK and new users a different reaction input format is available. A maximum of three reactants and four products (without stoichiometric coefficients) is allowed under this format.

For the reacting species, any combinations of letters and numbers can be used to identify the individual entries with the exception that the letter M is exclusively reserved to designate the total pressure and TEMP is reserved for the temperature.

To specify a "flow in" reaction, that is, the continuous addition of a particular species, a reaction with only products can be used where the reaction rate k is equal to the flow rate. A reaction with a reactant but no products implies a first-order "flow out" process.

When preparing the data, one must ensure that the rate constant is in units consistent with the order of the reaction as specified in the reaction mechanism. Instead of input of a rate constant for each photolysis reaction, a photolysis ratio is entered when variable photolysis is used (see the section on the General Data Card). This ratio is the ratio of the actual photolysis rate constant to the photolysis values entered on the card(s) following the General Data Card. For example, if the user inputs photolysis values, then each of the photolysis reactions will have a photolysis constant determined at each instant in time from the product of the interpolated photolysis value and the ratio entered on the reaction card. All photolysis values must be declared on the card after the General Data Card, as discussed earlier. Therefore, for example, if the photolysis values represent NO_2 photolysis rate constants, then the NO_2 photolysis reaction identification number must be declared and a value of 1.0 entered for the rate constant. It is also wise to keep in mind the following points:

- HO2 and HOO will be treated as different species.
- 2NO will be treated as a new species and not as two NOs unless the EPASIM format is used.
- The maximum number of different species is 89.

Title Card

Each simulation is titled by entering the desired notation in columns 1 through 28 of this card. Anything may be entered in the first four columns of this card with the following exceptions:

- All blank: This card will terminate the program.
- CONT: This is an option indicating that concentrations and species from a previous run will be used as initial conditions for a new run.
- MORE: This choice indicates that new reactions or new photolysis and temperature values are to be added.
- PLOT: This entry activates the plotting routine.

Output Specification Card

The first two items on this card specify the number of reactants with nonzero initial concentrations and the number of integration steps between print cycles. Normally, the program suppresses the printing of the concentrations of all species as a function of the integration steps. However, the user may key the output to the frequency of the integration steps by entering a negative number of steps between print-outs in the appropriate slot on the data card. Thus, if the user enters a value of -5, the program will print the instantaneous concentrations every 5 iteration steps. If the user only wants concentrations printed at specified intervals, then this option should not be activated (i.e. leave this slot blank). To obtain output at specific times, the user enters the initial print time and then either a fixed time increment or a fixed multiple to be used between subsequent printings. For example, a user may specify an initial

print time of 10 minutes and set the time increment at 10 minutes. In this case, output will be printed at 10 minutes, 20 minutes, 30 minutes, and so on. Or the user may specify an initial print time of 10 minutes and then set the print multiple at 2, in which case output is provided at 10 minutes, 20 minutes, 40 minutes, 80 minutes, and so on.

Initial Reactant Identification Card(s)

The vector containing the alphabetic designation of all reactants with a nonzero initial concentration is given on this card(s).

Initial Reactant Concentration Card(s)

The initial concentrations of all reactants, in appropriate units, are provided on this card in the same sequence as species are entered on the Initial Reactant Identification Card(s).

Time Specification Card

The simulation starting time and ending time are the first two arguments on this card. Their time unit should be identical to that used to specify rate constants. In addition, the absolute temperature and the error tolerance for the integration step may be entered on this card. Default values of these parameters are 298K and 10^{-2}, respectively.

After each simulation the user may choose the following options:

> Start a new simulation with the same mechanism by first inserting a new title card.
> Terminate the program by inserting a blank card.
> Provide a new or changed reaction sequence and start a new calculation using the MORE option.

Continue the calculation using the current results but with some parameter changed using the CONT option. Plot the computed output using the PLOT option.

All of these possibilities are discussed in the following section.

PROGRAM OPTIONS

More Than One Computation

Rather than enter a terminating blank card, insert a new title card followed by a new set of initial condition data. The new data will provide computational results using the previously specified reaction scheme.

To Continue with Previously Calculated Species

If the new title card has CONT in its first four columns, the species from the previous calculation and their concentrations will be used as initial conditions for a problem in which either new reactions are entered or the temperature or error tolerance is changed. The next card must in this case be the time specification card, having the starting and ending times, error tolerance, and temperature.

New or Changed Reactions

To introduce either new or changed reactions into the kinetic mechanism, enter a card with the word MORE punched in columes 1 through 4 followed by the set of cards used for specifying the changes in the kinetic mechanism. This set includes a first card similar to the General Data Card. Any parameter controlled on the original General Data Card can be changed on this new version. The difference between this card and the original is that all blank fields will default to the parameters controlled on the original card or to the present values changed by previous uses of

the MORE option. For example the dilution factor may be the only change desired. To accomplish this a MORE card followed by a card with only the new dilution factor in columns 21 through 30 would be used. The next card in this example might then be a CONT to continue the previous calculation or a new title to start an entirely new calculation with the same mechanism modified only by the new dilution factor.

The most frequent utilization of this option is typically for additions or alterations to the original mechanism. To alter any reaction a new reaction card is entered with the same identification number as the original. The new card must contain the complete reaction in its new form since it will replace the original. New reactions must have identification numbers not previously used in the original mechanism. In any case the identification number of the last reaction card to be read in at this time must appear on the new General Data Card in columns 1 to 3.

A new variable photolysis vector, a new variable temperature vector, or a new set of photolysis reactions controlled by the variable photolysis vector can also be introduced using this option. If a new photolysis reaction is to be added to the original set that varies with the time dependent photolysis vector, then the entire new set, including both the originals and the new additions, must be read in.

Plot Option Card

At the end of the computational cycle, a card with PLOT in its first four columns must be entered. This signals the program that the plot option is to be used and plot data are to follow.

Plot Title Card

If a plot has been selected by entering the word PLOT on the above card, then the user must supply a plot title card, which may have storage option

entry and an option to print the species concentrations at certain time steps. The storage option entry determines whether the plotted output will be stored on a tape file for later access. If the output is to be stored, the user need only insert any nonzero number in the option argument space.

The data is stored on a file titled TAPE 7 in unformatted form. The following parameters are written to the file TAPE 7:

> NTIT--The plot title.
> NAME(L)--The Lth species being plotted.
> CLOW--The lowest concentration entered on the plot specification card.
> CHIGH--The highest concentration value entered on the plot specification card.
> TLOW--The lowest time value entered on the plot specification card.
> THIGH--The highest time value entered on the plot specification card.
> NDAT--Number of observed data points.
> NPNT--Number of calculated data points.
> (TIME(J),J=1,NDAT)--The vector of time values of the observed data.
> (DATA(J),J=1,NDAT)--The vector of observed concentration values.
> (SAVTIM(J),J=1,NPNT)--The vector of time values of the calculated data.
> (SAVCON(L,J),J=1,NPNT)--The vector of calculated concentrations.

The twelve parameters are written with a single WRITE statement and should be read in the same manner.

If the user is interested in the actual concentrations of the species being plotted, then a nonzero value entered for this option will activate the

printing of the actual concentrations at the times closest to every one-eightieth of the total simulation time. Thus, if the total simulation time is 400 minutes then calculated concentrations at 5-minute intervals are printed.

Plot Specification Card

The plotting routine can handle up to three species on one plot. This is done by specifying the number of species to be plotted on the plot specification card. The information entered on this card is: The number of species to be plotted, the concentration labels for the vertical axis (five labels must be entered), the lowest and highest values of the concentrations, and the lowest and highest values of the integration time.

Species Information Card

This card contains the name of the species to be plotted (the species identification code), the number of data points to be plotted from experimental data, and the plot output symbol. If the number of experimental data points is zero, the next card is not entered. A species identification card must be entered for each species to be plotted.

Experimental Plot Data Cards

A unique feature of the PLOT program is its ability to overlay experimental data over a computer concentration profile. To do this, pairs of time and concentration values must be entered for each species. Four pairs of these values appear on each card, and the number of entries corresponds to the value specified on the previous data card.

End of Plot Data Card

A blank card must be entered to signal the end of the plot data. The next card can start a new simulation.

End of Program Card

A blank card entered instead of a new title or option card ends the program.

Table 1 provides an individual description of each data card, its argument list, format code, and column entries.

Calculation of the Round-Off Error

The variable UROUND in block data ALPHA1 should be set to the round-off error associated with each computer system. Currently, UROUND is set to the round-off error of 7.5×10^{-15} associated with a CDC 7600 computer system. To reset UROUND, the card (W.16) in block data ALPHA1 should be changed:

```
DATA      UROUND/user's round-off error/      (card W.16)
```

UROUND is calculated from the number of significant digits (N) used for the mantissa of a floating point constant:

$$\text{UROUND} = 2^{-N}$$

For example, on the UNIVAC 1110 computer, each word contains 36-BITs of which 27 are used for the mantissa. Thus, 2^{-27} is equal to approximately 7.5×10^{-9}. This is the value required for UROUND in CHEMK.

TABLE 1. INPUT CARD DESCRIPTION

Card	Column	Format	Description
General Data Card	1-3	I3	Last number of reaction sequence
	6-10	I5	Choice of reaction input format: Nonzero=EPASIM, default=CHEMK format
	11-14	A4	Print option for net rates of reaction and species rate of formation: default=printing is suppressed
	15-20	--	Not read
	21-30	F10.0	Dilution factor
	31-35	I5	Number of photolysis time units
	36-40	I5	Time interval of each photolysis time unit
	41-45	I5	Number of photolysis reactions
	46-50	I5	Number of temperature time units
	51-55	I5	Time interval of each temperature time unit
	56-60	--	Option to plot photolysis values as a function of time
	61-80	--	Not read
Next card(s)	1-10 11-20 21-30 . . . 61-70	7I10	If there are variable photolysis rate constants, the reaction identification vector identifying number of each photolysis reaction is read here
	71-80	--	Not read
Next card(s)	1-10 11-20 21-30 31-40 . . . 61-70	7F10.0	The initial photolysis and the value at the end of each time unit. If photolysis occurs for N units of time, then there should be N+1 photolysis values
	71-80	--	Not read

Table 1 (Continued)

Card	Column	Format	Description
Next card(s)	1-10 11-20 21-30 31-40 · · · 61-70	7F10.0	If variable temperature is used then the temperature values are read here. If there are N units of time in which the temperature changes, then there should N+1 temperature values
	71-80	--	Not read
Kinetic Mechanism Card (EPASIM format)	1-4, 7-11, 13-16,	A4 A4 A4	The names of the reactants (up to three are allowed)
	17-18	I2	The identification number of the reaction (number may be between 0 and 99; 0 only if next field is nonzero)
	19-23	F5.0	The stoichiometric coefficient of the first product; a blank implies a default value of 1
	24	I1	Modulus factor for reaction identification numbers greater than 100 (values are 0 or blank, 1, and 2); if a value of 1 is entered, the reaction identification number will be between 100 and 199 depending on the value in columns 17 and 18
	25-28	A4	The name of the first product
	32-36	F5.0	The stoichiometric coefficient of the second product
	37-40	A4	The name of the second product
	41-45	F5.0	The stoichiometric coefficient of the third product

Table 1 (Continued)

Card	Column	Format	Description
	49-52	A4	The name of the third product
	55-64	F10.0	The rate constant at 298K or, for photolysis reactions, the ratio of the photolysis value to reaction number 1
	66-72	F7.0	The activation energy in degrees Kelvin (K)
Kinetic Mechanism Card (CHEMK format)*	1- 3	I3	The reaction identification number
	6- 9 11-14 16-19	A4	The names of the reactants (up to three allowed)
	21-24 26-29 31-34 36-39	A4	The names of the products (up to four allowed)
	41-50	F10.0	The rate constant at 298K or the photolysis ratio for photolysis reactions
	51-60	F10.0	The activation energy in degrees Kelvin (K)
Title Card	1-72	18A4	The first four columns must not all be blank or contain one of the following: MORE, CONT, PLOT
Output Specification Card	1- 3	I3	Number of reactants with initial nonzero concentrations (maximum is 89)
	21-30	I10	Number of integration steps between print cycles; default is 10^4 to suppress printing keyed to step size.
	31-40	F10.0	Specific time of initial print (independent of step size)

TABLE 1 (Continued)

Card	Column	Format	Description
	41-50	F10.0	Time interval
	51-60	F10.0	Time multiple (note that at least one of the above two fields must be blank)
Initial Reactant Card(s)	1- 4, 11-14 21-24 • • • 61-64	A4	Alphanumeric identification of the reactants with initial nonzero concentrations seven species per card
	65-80	--	Not read
Initial Reactant Concentration Card(s)	1-10 11-20 21-30 • • 61-70	F10.0	Initial concentrations of reactants. Concentrations must be given in the same sequence as the species are given on Initial Reactant Card(s)
	71-80	--	Not read
Time Specification Card	1-10	F10.0	Simulation starting time. Time must be in the same units as the rate constants
	11-20	F10.0	Simulation ending time. Time must be in the same units as the rate constants
	21-30	F10.0	Temperature (constant throughout the simulation if variable temperature profile is not used; default=298K)
	31-40	F10.0	Error tolerance; default=10^{-2}
	41-80	--	Not read

TABLE 1 (Continued)

Card	Column	Format	Description
Options Card	1- 4	A4	Plot initiated if PLOT is entered. Additional kinetic steps are processed if MORE is entered. A new starting time is used if CONT is entered. Program terminates if blank card is inserted.
	5-80	--	Not read
Plot Option Cards:			
Plot Title	1-12	3A4	Title of simulation
	13-54	--	Not read
	55-60		Option to print actual concentrations of all plotted species
	61-65	I5	Data storage option. If nonzero, plot data is saved on a file named TAPE7
	66-80	--	Not read
Plot Specification Card	1- 5	--	Not read
	6- 7	I2	Number of species to be plotted; up to three species may be placed on one plot
	8-15	--	Not read
	16-19 21-24 26-29 31-34 36-39	A4	Concentration labels: Five arguments must be entered
	41-50	F10.0	Lowest concentration value
	51-60	F10.0	Highest concentration value
	61-70	F10.0	Lowest time value
	71-80	F10.0	Highest time value

TABLE 1 (Concluded)

Card	Column	Format	Description
Species Identification Card (one card for each species)	1 - 4	A4	Name of species to be plotted
	6- 7	I2	Number of data points to be plotted from experimental data. Value must be between 1 and 80. If set at zero, no experimental data are read
	8	--	Not read
	9	A1	Symbol for plotted output
	10-80	--	Not read
Experimental Plot Data	1-10	F10.0	Time
	11-20	F10.0	Concentration
	21-30 31-40 . . . 61-70, 71-80	F10.0	(A total of four sets of time and concentration are placed on each card)
End of Plot Data	1- 4	A4	Blank card
	5-80	--	Not read
End of Program	1- 4	A4	Blank card
	5-80	--	Not read

* Default reaction format

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Appendix A
Program Listing

```
                                                                      A    3
C*************************************************************************A    4
C                                                                     A    5
C     CHEMK IS A FORTRAN PROGRAM WHICH, WHEN GIVEN A PREDETERMINED    A    6
C     KINETIC MECHANISM, COMPUTES THE CONCENTRATIONS OF THE VARIOUS   A    7
C     REACTANTS IN TIME. IT WAS WRITTEN BY GARY Z. WHITTEN OF SYSTEMS A    8
C     APPLICATIONS INCORPORATED IN SAN RAFAEL, CA AND INCORPORATES    A    9
C     THE GEAR INTEGRATION PACKAGE OF A. HINDMARSH OF LAWRENCE LIVERMORE A   10
C     LABORATORIES IN LIVERMORE, CA.  THE PRINTER-PLOT ROUTINE WAS    A   11
C     PROVIDED BY DAVID C. WHITNEY OF SAI AND THE PROGRAM WAS CONVERTED A   12
C     ANSI FORTRAN BY JIM MEYER OF SAI. THE  COMPUTER CODE THAT FOLLOWS A   13
C     IS EXECUTABLE ON ANY IBM OR CDC MACHINE WITH A FORTRAN IV COMPILER A  14
C                                                                     A   15
C     TWO SEPARATE SETS OF DATA ARE NEEDED TO EXECUTE THE PROGRAM. ONE A   16
C     SET CONTROLS THE COMPUTATIONAL PART OF THE PROGRAM AND IS       A   17
C     NECESSARY TO ESTABLISH THE INTEGRATION ROUTINE.  THE SECOND SET OF A  18
C     CONTROLS THE PLOTTER OUTPUT AND PROVIDES THE PARAMETERS NECESSARY A   19
C     SPECIFY THE  OUTPUT FORMAT.  THE READER IS REFERED TO THE PROGRAM A   20
C     FOR FURTHER INFORMATION.                                        A   21
C                                                                     A   22
C                                GARY Z. WHITTEN                      A   23
C                                SYSTEMS APPLICATIONS INCORPORATED    A   24
C                                950 NORTHGATE DRIVE                  A   25
C                                SAN RAFAEL, CALIFORNIA  94903        A   26
C                                (415) 472-4011                       A   27
C                                                                     A   28
C*************************************************************************A   29
C                                                                     A   30
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START, A   31
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT        A   32
      COMMON /NAMES/ SPECIS(91),REACT(91),NS                          A   33
      COMMON /FRPLOT/ NIT(3),SAVCON(90,80),SAVTIM(80),JGRID(89,40),NT A   34
      COMMON /ALPHA/ IGO(4),IBLANK,MBLANK,JINTER                      A   35
      COMMON /APLOT/ JVERT(52,2),JBLANK,JSTAR,JPLUS,JBAR              A   36
      COMMON /GEAR1/ T,GUESS,HMIN,HMAX,EPS1,UROUND,NC,MF1,KFLAG1,JSTART A   37
      COMMON /GEAR2/ YMAX(100)                                        A   38
      COMMON /INOUT/ IN,IOUT,ITAPE                                    A   39
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP              A   40
      COMMON /SPARSE/ IA(91),JA(1000)                                 A   41
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST, A   42
     1IPH(30),QM(100),PM(100),PSTOP                                   A   43
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10                   A   44
      DIMENSION C(91), IRS(200,7), KRS(7), SC1(7)                     A   45
      INTEGER SPECIS,REACT,PHI,TMI,AST                                A   46
C                                                                     A   47
C     ALPHAMERIC DATA ARE PREASSIGNED IN BLOCK DATA ALPHA1            A   48
C                                                                     A   49
      DATA NPLOT/4HSAVE/,IBLK/1H /                                    A   50
      DATA IN2,IN3,IN5,IN6,IN7,IN8,IN9/7*1/                           A   51
      DATA XN4,XN6,XN9/3*1.0/                                         A   52
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```
C                                                                       A  53
C     INITIAL PARAMETERS                                                A  54
C                                                                       A  55
      IN=5                                                              A  56
      IOUT=6                                                            A  57
      ITAPE=7                                                           A  58
C                                                                       A  59
C     CLEAR PATTERN MATRIX AND SET THE FIRST ELEMENTS                   A  60
C     ALSO SET STOICHIOMETRIC COEFFICIENTS EQUAL TO 1                   A  61
C                                                                       A  62
      DO 5 J=1,200                                                      A  63
      DO 5 K=1,7                                                        A  64
      IRS(J,K)=IBLANK                                                   A  65
      SC(J,K)=1.                                                        A  66
    5 KR(J,K)=0                                                         A  67
      DO 10 J=1,200                                                     A  68
      A(J)=0.                                                           A  69
      R(J)=0.                                                           A  70
   10 S(J)=0.                                                           A  71
      NR=0                                                              A  72
      NS=0                                                              A  73
C                                                                       A  74
C     NX = LAST NUMBER OF THE REACTION SEQUENCE                         A  75
C     NPLOT = PLOT OPTION                                               A  76
C     DILUT= DILUTION FACTOR                                            A  77
C                                                                       A  78
      READ (IN,185) NX,NEPA,NPLIT,DILUT,NPHOT,PHI,IL,NTEMP,TMI,IPP     A  79
      GO TO 20                                                          A  80
   15 NS=NS-1                                                           A  81
      READ (IN,185) NX,IN2,IN3,XN4,IN5,IN6,IN7,IN8,IN9,IN10             A  82
      IF (IABS(IN2).NE.0) NEPA=IN2                                      A  83
      NPLIT=IN3                                                         A  84
      IF (ABS(XN4).NE.0) DILUT=XN4                                      A  85
      IF (IABS(IN5).NE.0) NPHOT=IN5                                     A  86
      IF (IABS(IN6).NE.0) PHI=IN6                                       A  87
      IF (IABS(IN7).NE.0) IL=IN7                                        A  88
      IF (IABS(IN8).NE.0) NTEMP=IN8                                     A  89
      IF (IABS(IN9).NE.0) TMI=IN9                                       A  90
      IF (IABS(IN10).NE.0) IPP=IN10                                     A  91
   20 IF (IL.LE.0.OR.IN7.LE.0) GO TO 25                                 A  92
      READ (IN,200) (IPH(I),I=1,IL)                                     A  93
   25 IF (NPHOT.LE.0.OR.IN5.LE.0) GO TO 30                              A  94
      NPHOT=NPHOT+1                                                     A  95
      READ (IN,190) (PM(I),I=1,NPHOT)                                   A  96
      PM(NPHOT+1)=2.0*PM(NPHOT)-PM(NPHOT-1)                             A  97
      PM(NPHOT+2)=3.0*PM(NPHOT)-2.0*PM(NPHOT-1)                         A  98
      PSTOP=FLOAT((NPHOT-1)*PHI)                                        A  99
   30 IF (NTEMP.LE.0.OR.IN8.LE.0) GO TO 35                              A 100
      NTEMP=NTEMP+1                                                     A 101
      READ (IN,190) (QM(I),I=1,NTEMP)                                   A 102
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```
      QM(NTEMP+1)=2.*QM(NTEMP)-QM(NTEMP-1)                                A 103
      QM(NTEMP+2)=3.0*QM(NTEMP)-2.0*QM(NTEMP-1)                           A 104
      TEMEND=FLOAT((NTEMP-1)*TMI)                                         A 105
   35 IF (NX.GT.0) WRITE (IOUT,130)                                       A 106
      IF (NX.LE.0) NS=NS+1                                                A 107
      IF (NX.LE.0) GO TO 80                                               A 108
C                                                                         A 109
C     REACTION INPUT DATA                                                 A 110
C                                                                         A 111
   40 IF (NEPA.LE.0) READ (IN,135) J,(IRS(J,I),I=1,7),A(J),S(J)           A 112
      IF (NEPA.LE.0) GO TO 55                                             A 113
      READ (IN,220) (KRS(I),I=1,3),J,SC1(1),JJ,KRS(4),(SC1(LL-3),KRS(LL) A 114
     1,LL=5,6),RTE,ENERGY                                                 A 115
      IF (JJ.GT.0) J=JJ*100+J                                             A 116
      DO 45 II=1,6                                                        A 117
   45 IRS(J,II)=KRS(II)                                                   A 118
      A(J)=RTE                                                            A 119
      S(J)=ENERGY                                                         A 120
      DO 50 II=4,6                                                        A 121
   50 SC(J,II)=SC1(II-3)                                                  A 122
   55 DO 60 I=1,7                                                         A 123
   60 IF (SC(J,I).LE.0.) SC(J,I)=1.                                       A 124
      DO 75 K=1,7                                                         A 125
      NL=K*5                                                              A 126
      NF=NL-4                                                             A 127
      DO 65 LK=NF,NL                                                      A 128
   65 AST(LK)=IBLK                                                        A 129
      IPL(K)=IBLK                                                         A 130
      IF (K.EQ.1.OR.K.EQ.4) GO TO 70                                      A 131
      IF (IRS(J,K).NE.IBLANK) IPL(K-1)=JPLUS                              A 132
   70 IF (IRS(J,K).NE.IBLANK) CALL VALU (SC(J,K),K,NF,NL)                 A 133
   75 CONTINUE                                                            A 134
      WRITE (IOUT,140) J,(AST(I),I=1,5),IRS(J,1),IPL(1),(AST(I),I=6,10), A 135
     1IRS(J,2),IPL(2),(AST(I),I=11,15),IRS(J,3),IPL(3),(AST(I),I=16,20), A 136
     2IRS(J,4),IPL(4),(AST(I),I=21,25),IRS(J,5),IPL(5),(AST(I),I=26,30), A 137
     3IRS(J,6),IPL(6),(AST(I),I=31,35),IRS(J,7),IPL(7),A(J),S(J)         A 138
      KR(J,1)=100                                                         A 139
      IF (J.GT.NR) NR=J                                                   A 140
      IF (J.NE.NX) GO TO 40                                               A 141
C                                                                         A 142
C     ESTABLISH REACTION MATRIX AND SET UP SPARSE JACOBIAN VECTORS        A 143
C                                                                         A 144
      CALL MATRX (C,IRS)                                                  A 145
      CALL SPARS (IA,JA,NS-2)                                             A 146
      INX=1                                                               A 147
C                                                                         A 148
C     TITLE CARD AND OPTIONS                                              A 149
C                                                                         A 150
   80 READ (IN,195) (ITITLE(I),I=1,7)                                     A 151
      NFL=0                                                               A 152
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```
      IF (ITITLE(1).EQ.IGO(1)) GO TO 15                                  A  153
      IF (ITITLE(1).EQ.IGO(2)) GO TO 115                                 A  154
      IF (ITITLE(1).EQ.IGO(3)) GO TO 85                                  A  155
      IF (ITITLE(1).EQ.IBLANK) STOP                                      A  156
      GO TO 90                                                           A  157
C                                                                        A  158
C     CALL PLOT                                                          A  159
C                                                                        A  160
   85 READ (IN,180) (NIT(I),I=1,3),IDT,KALCMP                            A  161
      NT=NT-2                                                            A  162
      CALL PLOT (NIT,NT,NS,SPECIS,SAVTIM,SAVCON,IDT,KALCMP,JGRID)        A  163
      GO TO 80                                                           A  164
C                                                                        A  165
C     OPTIONS CARD                                                       A  166
C                                                                        A  167
   90 READ (IN,155) N,NPRNT,TPRNT,TSTEP,TFACT                            A  168
C                                                                        A  169
C     TIME STEP SKIP OPTION                                              A  170
C                                                                        A  171
      IF (NPRNT*NPRNT.EQ.0) NPRNT=100000                                 A  172
C                                                                        A  173
C     TIME STEP LENGTH OPTION                                            A  174
C                                                                        A  175
      IF (TPRNT*TPRNT.EQ.0.) TPRNT=1.E10                                 A  176
C                                                                        A  177
C     CONCENTRATION OF SPECIES INITIALLY PRESENT                         A  178
C                                                                        A  179
      READ (IN,125) (REACT(I),I=1,N)                                     A  180
      READ (IN,190) (C(I),I=1,N)                                         A  181
C                                                                        A  182
C     STARTING AND ENDING INTEGRATION TIMES                              A  183
C                                                                        A  184
      READ (IN,175) START,STOPP,TEMP,ERR                                 A  185
      IF (START*START.EQ.0.) START=0.                                    A  186
C                                                                        A  187
C     SPECIFICATION OF THE TEMPERATURE IF UNSPECIFIED IN INPUT           A  188
C                                                                        A  189
      IF (TEMP.LE.0.) TEMP=298.                                          A  190
C                                                                        A  191
C     SPECIFICATION OF THE ERROR BOUND IF UNSPECIFIED IN INPUT           A  192
C                                                                        A  193
      IF (ERR*ERR.EQ.0.) ERR=1.E-2                                       A  194
C                                                                        A  195
C     OUTPUT OF THE INITIAL CONDITIONS                                   A  196
C                                                                        A  197
      WRITE (IOUT,145) (ITITLE(I),I=1,7),(REACT(I),I=1,N)                A  198
   95 WRITE (IOUT,150) (C(I),I=1,N)                                      A  199
C                                                                        A  200
C     COMPUTE THE NET RATES OF REACTION                                  A  201
C                                                                        A  202
```

```
      IF (NTEMP.GT.0) TEMP=QM(1)                                    A 203
      IF (ITITLE(1).EQ.IGO(2).AND.NTEMP.GT.0) TEMP=TEMOLD           A 204
      CALL RATES (C,N)                                              A 205
C                                                                   A 206
C     OUTPUT OF THE TEMPERATURE AND ERROR BOUND                     A 207
C                                                                   A 208
      WRITE (IOUT,160) TEMP,ERR                                     A 209
C                                                                   A 210
C     OUTPUT OF THE DILUTION FACTOR                                 A 211
C                                                                   A 212
      IF (DILUT*DILUT.EQ.0.) DILUT=0.                               A 213
      IF (DILUT.NE.0.) WRITE (IOUT,170) DILUT                       A 214
C                                                                   A 215
C     SET LIMITS FOR TIMED OUTPUTS                                  A 216
C                                                                   A 217
      IF (TSTEP.NE.0.) YMAX(1)=TSTEP                                A 218
      IF (TSTEP.NE.0.) PC=TSTEP                                     A 219
      IF (TSTEP*TSTEP.EQ.0.) YMAX(1)=1.E10                          A 220
      IF (TSTEP*TSTEP.EQ.0.) PC=1.E10                               A 221
      IF (TFACT.NE.0.) YMAX(2)=TFACT                                A 222
      IF (TFACT*TFACT.EQ.0.) YMAX(2)=1.                             A 223
C                                                                   A 224
C     RATE CONSTANTS                                                A 225
C                                                                   A 226
      WRITE (IOUT,165) (R(I),I=1,NR)                                A 227
C                                                                   A 228
C     WRITE INITIAL CONDITIONS OF THE CELL                          A 229
C                                                                   A 230
      IF (NPHOT.LE.0) GO TO 105                                     A 231
      WRITE (IOUT,215) (IPH(I),I=1,IL)                              A 232
      DO 100 I=1,IL                                                 A 233
      J=IPH(I)                                                      A 234
      YMAX(10+I)=R(J)                                               A 235
  100 CONTINUE                                                      A 236
      WRITE (IOUT,225) (YMAX(10+I),I=1,IL)                          A 237
      NPT=NPHOT                                                     A 238
      WRITE (IOUT,205) PHI,(PM(I),I=1,NPT)                          A 239
  105 IF (NTEMP.LE.0) GO TO 110                                     A 240
      NPT=NTEMP                                                     A 241
      WRITE (IOUT,210) TMI,(QM(I),I=1,NPT)                          A 242
  110 GUESS=1.E-10                                                  A 243
      T=START                                                       A 244
      IF (NPLOT.EQ.IBLANK) YMAX(3)=0.                               A 245
      IF (NPLOT.NE.IBLANK) YMAX(3)=1.                               A 246
      IF (NPLIT.NE.IBLANK) YMAX(4)=1.                               A 247
      IF (NPLIT.EQ.IBLANK) YMAX(4)=0.                               A 248
C                                                                   A 249
C     INITIALIZE PARAMETERS                                         A 250
C                                                                   A 251
      CALL YFIX (NS,TPRNT,C,NPRNT,INX)                              A 252
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```
      INX=4                                                              A  253
      TEMOLD=TEMP                                                        A  254
      GO TO 80                                                           A  255
C                                                                        A  256
C     CONTINUATION OF DATA                                               A  257
C                                                                        A  258
  115 READ (IN,175) START,STOPP,TEMP,ERR                                 A  259
      IF (TEMP.LE.0.) TEMP=298.                                          A  260
      IF (TEMOLD.NE.298..AND.TEMOLD.NE.0.) TEMP=TEMOLD                   A  261
      IF (ERR*ERR.EQ.0.) ERR=1.E-2                                       A  262
      DO 120 I=1,NS                                                      A  263
  120 REACT(I)=SPECIS(I)                                                 A  264
C                                                                        A  265
C     INITIAL CONDITIONS                                                 A  266
C                                                                        A  267
      WRITE (IOUT,145) (ITITLE(I),I=1,7),(REACT(I),I=1,NS)               A  268
      N=NS                                                               A  269
      GO TO 95                                                           A  270
C                                                                        A  271
C                                                                        A  272
  125 FORMAT (7(A4,6X))                                                  A  273
  130 FORMAT (1H1,14H THE REACTIONS,86X,13HRATE CONSTANT,2X,15HACT. ENER A  274
     1GY (K))                                                            A  275
  135 FORMAT (I3,2X,7(A4,1X),2F10.0)                                     A  276
  140 FORMAT (/,2X,I3,2X,3(5A1,1X,A4,2X,A1),1H=,2X,4(5A1,1X,A4,2X,A1),1P A  277
     1E11.3,2X,E13.3)                                                    A  278
  145 FORMAT (1H1,30X,7A4,//,23H INITIAL CONCENTRATION ,//(10X,10(4X,A4, A  279
     14X)))                                                              A  280
  150 FORMAT (/(8X,1P10E12.3))                                           A  281
  155 FORMAT (I3,17X,I6,4X,3F10.0)                                       A  282
  160 FORMAT (/,34H THE TEMPERATURE OF THE CELL WAS =,1PE9.2,26H AND THE A  283
     1 ERROR TOLERANCE =,E9.2)                                           A  284
  165 FORMAT (/,29H THE RATE CONSTANTS USED WERE,/,(/,8X,1P10E12.3))     A  285
  170 FORMAT (/,30H THE OVERALL DILUTION RATE WAS,1PE9.2)                A  286
  175 FORMAT (8F10.0)                                                    A  287
  180 FORMAT (3A4,43X,2I5)                                               A  288
  185 FORMAT (I3,2X,I5,A4,6X,F10.2,6I5)                                  A  289
  190 FORMAT (7F10.3)                                                    A  290
  195 FORMAT (7A4)                                                       A  291
  200 FORMAT (7I10)                                                      A  292
  205 FORMAT (/44HOTHE NO2 PHOTOLYSIS NUMBERS IN INTERVALS OF ,I3,15H TI A  293
     1ME UNITS ARE,/,(1HO,1P10E13.3))                                    A  294
  210 FORMAT (/34HOTHE TEMPERATURES IN INTERVALS OF ,I3,15H TIME UNITS A A  295
     1RE/(1HO,1P10E13.3))                                                A  296
  215 FORMAT (/29HOTHE PHOTOLYSIS REACTIONS ARE,/(1HO,9I13))             A  297
  220 FORMAT (2(A4,2X),A4,I2,F5.1,I1,A4,2X,2(F5.0,1X,A4,2X),F10.2,1X,F7. A  298
     12)                                                                 A  299
  225 FORMAT (57HOTHE PHOTOLYSIS RATIOS OF EACH OF THE REACTIONS ABOVE A A  300
     1RE/(1HO,4X,1P9E13.3))                                              A  301
      END                                                                A  302-
```

```
      SUBROUTINE YFIX (NO,TLAST,C,NQ,INDEX)                                  B    1
                                                                             B    2
C*****************************************************************************B    3
                                                                             B    4
C     THIS IS THE NORMAL OUTPUT ROUTINE                                      B    5
                                                                             B    6
C*****************************************************************************B    7
                                                                             B    8
      COMMON /SPARSE/ IA(91),JA(1000)                                        B    9
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,     B   10
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT               B   11
      COMMON /NAMES/ SPECIS(91),REACT(91),NS                                 B   12
      COMMON /FRPLOT/ NIT(3),SAVCON(90,80),SAVTIM(80),JGRID(89,40),NT        B   13
      COMMON /GEAR1/ D,H,DUM(4),IDUM(4)                                      B   14
      COMMON /GEAR2/ YMAX(100)                                               B   15
      COMMON /INOUT/ INPP,IOUT,ITAPE                                         B   16
      COMMON /HEAT/ CV,O(200),SC(200,7),ISC(200,3),ITEMP                     B   17
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST,     B   18
     1IPH(30),QM(100),PM(100),PSTOP                                          B   19
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10                          B   20
      DIMENSION C(91), RT(200)                                               B   21
      INTEGER SPECIS,REACT,TMI,PHI,AST                                       B   22
      DATA IGO/4HCONT/                                                       B   23
      DATA NT1/1/                                                            B   24
      DATA START1/0.0/                                                       B   25
      N=NS-1                                                                 B   26
      NS2=NS-2                                                               B   27
      NFRST=1                                                                B   28
                                                                             B   29
C     TIME INTERVALS                                                         B   30
                                                                             B   31
      IF (ITITLE(1).NE.IGO) GO TO 30                                         B   32
      IF (NT1.EQ.0) GO TO 30                                                 B   33
      TDC=(STOPP-START1)/80.                                                 B   34
      TD=START1+TDC                                                          B   35
      J=0                                                                    B   36
      NTSV=NT                                                                B   37
      DO 25 I=1,80                                                           B   38
    5 J=J+1                                                                  B   39
      IF (J.GT.NTSV) GO TO 20                                                B   40
      IF (SAVTIM(J).GE.TD) GO TO 10                                          B   41
      GO TO 5                                                                B   42
   10 SAVTIM(I)=SAVTIM(J)                                                    B   43
      DO 15 K=1,NS                                                           B   44
   15 SAVCON(K,I)=SAVCON(K,J)                                                B   45
      NT=I                                                                   B   46
      GO TO 25                                                               B   47
   20 IF (I.EQ.1) NT=1                                                       B   48
      SAVTIM(I)=TD                                                           B   49
   25 TD=TD+TDC                                                              B   50
```

```
      GO TO 40                                                          B   51
   30 TDC=(STOPP-START)/80.                                             B   52
      TD=START                                                          B   53
      DO 35 I=1,80                                                      B   54
      TD=TD+TDC                                                         B   55
   35 SAVTIM(I)=TD                                                      B   56
      START1=START                                                      B   57
      NT=1                                                              B   58
   40 NC=0                                                              B   59
C                                                                       B   60
C     INITIALIZE PARAMETERS                                             B   61
C                                                                       B   62
      NHS=0                                                             B   63
      MS=IABS(NQ)                                                       B   64
      TPRNT=TLAST+START                                                 B   65
      TSTEP=PC                                                          B   66
      TFACT=YMAX(2)                                                     B   67
      IF (TFACT.GT.1.) TSTEP=0.                                         B   68
      MT=50-((NS-1)/10)*3-(NR-1)/10                                     B   69
      NN=NS+1-MINO(NS/10,1)                                             B   70
      IF (YMAX(3).EQ.0.) NPLOT=0                                        B   71
      IF (YMAX(3).NE.0.) NPLOT=1                                        B   72
      IF (YMAX(4).EQ.0.) NOPT=0                                         B   73
      IF (YMAX(4).NE.0.) NOPT=1                                         B   74
      IF (NOPT.EQ.0) MT=50-((NS-1)/10)*2                                B   75
      NTP=0                                                             B   76
      NT1=NPLOT                                                         B   77
      IF (NPLOT.EQ.0) NT=-1                                             B   78
      IN=INDEX                                                          B   79
      T=START                                                           B   80
      TNEXT=START+1.                                                    B   81
      CALL DIFFUN (NS2,TNEXT,C,RT)                                      B   82
      CALL SAVLIN (T,C,NS2)                                             B   83
      NFRST=2                                                           B   84
      IF (T-START) 60,60,50                                             B   85
   45 TNEXT=AMIN1(TPRNT,STOPP)                                          B   86
      IF (T.EQ.START) GO TO 55                                          B   87
   50 IF (NQ.LT.0.AND.IABS(NQ).NE.0) IN=3                               B   88
   55 CALL DRIVES (NS2,T,H,C,TNEXT,ERR,21,IN,IA,JA)                     B   89
      T=TNEXT                                                           B   90
      IF (T.GE.STOPP) TPRNT=STOPP                                       B   91
   60 IF (T.EQ.START) TIMNW=START                                       B   92
      IF (T.NE.START) TIMNW=TPRNT                                       B   93
      IF (T.EQ.START) GO TO 65                                          B   94
      IF (NQ.LT.0.AND.IABS(NQ).NE.0) TIMNW=T                            B   95
      NHS=NHS+1                                                         B   96
      IF (NHS.GE.MS.OR.T.GE.TPRNT) GO TO 65                             B   97
      GO TO 45                                                          B   98
   65 NHS=0                                                             B   99
      CALL DIFFUN (NS2,TIMNW,C,RT)                                      B  100
```

```
      IF (NOPT.LE.0) NTP=NTP+(N/10)+4                                    B  101
      IF (NOPT.GT.0) NTP=NTP+(N/10)*3+(NR-1)/10+12                       B  102
      IF (NTP.GT.MT.OR.T.EQ.START) WRITE (IOUT,120)                      B  103
      IF (T.EQ.START) GO TO 70                                           B  104
      IF (NOPT.LE.0.AND.NTP.LE.MT) GO TO 75                              B  105
   70 CONTINUE                                                           B  106
      IF (NTP.GT.MT) NTP=0                                               B  107
      IF (NN.GE.11) WRITE (IOUT,115) (SPECIS(I),I=1,NN)                  B  108
      IF (NN.LE.10) WRITE (IOUT,125) (SPECIS(I),I=1,NN)                  B  109
   75 CONTINUE                                                           B  110
      IF (NS.GE.11) WRITE (IOUT,130) TIMNW,(C(I),I=1,10),H,(C(I),I=11,NS B  111
     12),TEMP,SG                                                         B  112
      IF (NS.LE.10) WRITE (IOUT,130) TIMNW,(C(I),I=1,NS2),TEMP,SG,H      B  113
      IF (NOPT.EQ.0) WRITE (IOUT,135)                                    B  114
      IF (NOPT.EQ.0) GO TO 95                                            B  115
      RT(NS)=0.                                                          B  116
      RT(N)=0.                                                           B  117
      DO 80 I=1,NS2                                                      B  118
   80 RT(NS)=RT(NS)+RT(I)                                                B  119
      WRITE (IOUT,105) (RT(I),I=1,NS)                                    B  120
      DO 90 I=1,NR                                                       B  121
      J=KR(I,1)                                                          B  122
      IF (J.EQ.0) RT(I)=0.                                               B  123
      IF (J.EQ.0) GO TO 90                                               B  124
      JT=ITYPE(I)                                                        B  125
      XT=1.                                                              B  126
      DO 85 L=1,JT                                                       B  127
      J=KR(I,L)                                                          B  128
      XJ=1.                                                              B  129
      IF (J.GT.0.AND.J.LE.NS2) XJ=C(J)**ISC(I,L)                         B  130
      IF (ISC(I,L).EQ.-1) XJ=C(J)**SC(I,L)                               B  131
      IF (J.EQ.NS) XJ=SG                                                 B  132
      XT=XT*XJ                                                           B  133
   85 CONTINUE                                                           B  134
      RT(I)=XT*R(I)                                                      B  135
   90 CONTINUE                                                           B  136
      WRITE (IOUT,110) (RT(I),I=1,NR)                                    B  137
   95 IF (TIMNW.EQ.START) GO TO 55                                       B  138
      IF (T.GE.STOPP) RETURN                                             B  139
      IF (IN.EQ.3.AND.T.LT.TPRNT) GO TO 45                               B  140
      TPRNT=TPRNT*TFACT+TSTEP                                            B  141
      GO TO 45                                                           B  142
C                                                                        B  143
C                                                                        B  144
  105 FORMAT (/,10H NET RATES,2X,1P10E12.3,/,(12X,1P10E12.3))            B  145
  110 FORMAT (//,2X,22HTHE REACTION RATES ARE,/,(1H ,1P10E13.2))         B  146
  115 FORMAT (/,4X,5HTIME ,4X,10(4X,A4,4X),/,2X,8HINTERVAL,3X,10(4X,A4,4 B  147
     1X),/,(13X,10(4X,A4,4X)))                                           B  148
  120 FORMAT (1H1)                                                       B  149
  125 FORMAT (/,4X,5HTIME ,4X,10(4X,A4,4X),/)                            B  150
```

```
130 FORMAT (/,1P11E12.3/,11E12.3/,(12X,10E12.3))                    B  151
135 FORMAT (1H )                                                    B  152
    END                                                             B  153-
```

```
      SUBROUTINE RATES (C,N)                                                C    1
C                                                                           C    2
C*************************************************************************** C    3
C                                                                           C    4
C     THIS SUBROUTINE SETS THE INITIAL CONCENTRATIONS AND CALCULATES THE    C    5
C     RATE CONSTANTS                                                        C    6
C                                                                           C    7
C*************************************************************************** C    8
C                                                                           C    9
      INTEGER SPECIS,REACT                                                  C   10
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,    C   11
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT              C   12
      COMMON /NAMES/ SPECIS(91),REACT(91),NS                                C   13
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP                    C   14
      COMMON /ALPHA/ IGO(4),IBLANK,MBLANK,JINTER                            C   15
      DIMENSION C(91)                                                       C   16
      FCT=1./298.-1./TEMP                                                   C   17
      SIGG=0.                                                               C   18
      DO 5 I=1,91                                                           C   19
    5 SIG(I)=0.                                                             C   20
      DO 15 I=1,N                                                           C   21
      DO 10 J=1,NS                                                          C   22
      IF (SPECIS(J).EQ.REACT(I)) SIG(J)=C(I)                                C   23
      IF (SPECIS(J).EQ.REACT(I)) GO TO 15                                   C   24
   10 CONTINUE                                                              C   25
      SIGG=SIGG+C(I)                                                        C   26
   15 CONTINUE                                                              C   27
      N=NS                                                                  C   28
      M=N-1                                                                 C   29
      C(N)=0.                                                               C   30
      DO 20 I=1,M                                                           C   31
      C(N)=C(N)+SIG(I)                                                      C   32
   20 C(I)=SIG(I)                                                           C   33
      BK=0.                                                                 C   34
C                                                                           C   35
C     IF SIG(N) DOES NOT EQUAL ZERO, IT IMPLIES THAT THAT THE CONCENTRAT    C   36
C     SPECIES N HAS BEEN READ. OTHERWISE M IS THE SUM OF THE INITIAL        C   37
C     CONCENTRATIONS.                                                       C   38
C                                                                           C   39
      C(N)=C(N)+SIGG                                                        C   40
      IF (SIG(N).NE.0.) BK=SIG(N)-C(N)                                      C   41
      IF (SIG(N).NE.0.) C(N)=SIG(N)                                         C   42
      NP=0                                                                  C   43
      DO 25 I=1,NR                                                          C   44
      IF (KR(I,1).EQ.0) GO TO 25                                            C   45
C                                                                           C   46
C     CALCULATE THE RATE CONSTANTS                                          C   47
C                                                                           C   48
      IF (ABS(S(I)).EQ.0.) R(I)=A(I)                                        C   49
      IF (ABS(S(I)).NE.0.) R(I)=A(I)*EXP(S(I)*FCT)                          C   50
```

```
25 CONTINUE                                                          C  51
   IF (NS.LE.9) SPECIS(NS+1)=JINTER                                  C  52
   RETURN                                                            C  53
   END                                                               C  54-
```

```
      SUBROUTINE DIFFUN (N,T,X,XT)                                          D    1
C                                                                           D    2
C*************************************************************************  D    3
C                                                                           D    4
C     THIS SUBROUTINE CALCULATES THE DERIVATIVE VECTOR OF THE ODE!S         D    5
C                                                                           D    6
C*************************************************************************  D    7
C                                                                           D    8
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,    D    9
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT              D   10
      COMMON /NAMES/ SPECIS(91),REACT(91),NS                                D   11
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP                    D   12
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST,    D   13
     1IPH(30),QM(100),PM(100),PSTOP                                         D   14
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),R1,IN10                          D   15
      DIMENSION XT(N), X(N)                                                 D   16
      INTEGER PHI,TMI                                                       D   17
      INTEGER SPECIS                                                        D   18
      P=BK                                                                  D   19
      DO 5 I=1,N                                                            D   20
      XT(I)=-DILUT*X(I)                                                     D   21
    5 P=P+X(I)                                                              D   22
      SG=P                                                                  D   23
      IF (NFRST.EQ.1) FCT=((3355.7046E-6)*TEMP-1.)/TEMP                     D   24
      IF (NFRST.EQ.1) GO TO 10                                              D   25
      IF (T.EQ.TOLD) GO TO 30                                               D   26
      IF (T.LE.1.) GO TO 30                                                 D   27
   10 IF (NPHOT.LE.0) GO TO 30                                              D   28
      IF (NFRST.NE.1) GO TO 15                                              D   29
      PINT=FLOAT(PHI)                                                       D   30
      PINV=1./PINT                                                          D   31
   15 CONTINUE                                                              D   32
      IF (T.GT.PSTOP) GO TO 20                                              D   33
      IZ=IFIX(T*PINV)+1                                                     D   34
      Z=T*PINV-FLOAT(IZ-1)                                                  D   35
      IF (T.LE.PINT) R1=PM(1)+(0.5*PM(3)*(Z-1.)+0.5*PM(1)*(Z-3.)-PM(2)*(    D   36
     1Z-2.))*Z                                                              D   37
      IF (T.LE.PINT) GO TO 20                                               D   38
      R1=PM(IZ)+0.25*Z*(5.*PM(IZ+1)-3.0*PM(IZ)-PM(IZ-1)-PM(IZ+2)+(PM(IZ-    D   39
     11)-PM(IZ)-PM(IZ+1)+PM(IZ+2))*Z)                                       D   40
   20 IF (R1.LT.0.) R1=0.                                                   D   41
      DO 25 IK=1,IL                                                         D   42
      IR=IPH(IK)                                                            D   43
      R(IR)=R1*A(IR)                                                        D   44
   25 IF (R(IR).LT.0.) R(IR)=0.                                             D   45
   30 TNOW=TEMP                                                             D   46
      IF (NFRST.EQ.1) GO TO 35                                              D   47
      IF (T.EQ.TOLD) GO TO 50                                               D   48
      IF (T.LE.1.) GO TO 50                                                 D   49
   35 CONTINUE                                                              D   50
```

```
      IF (T.GT.TEMEND) GO TO 50                                          D   51
      IF (NFRST.NE.1) GO TO 40                                           D   52
      TINT=FLOAT(TMI)                                                    D   53
      TINV=1./TINT                                                       D   54
   40 CONTINUE                                                           D   55
      IZ=IFIX(T*TINV)+1                                                  D   56
      Z=T*TINV-FLOAT(IZ-1)                                               D   57
      IF (T.LE.TINT) TNOW=QM(1)+(0.5*QM(3)*(Z-1.)+0.5*QM(1)*(Z-3.)-QM(2) D   58
     1*(Z-2.))*Z                                                         D   59
      IF (T.LE.TINT) GO TO 45                                            D   60
      TNOW=QM(IZ)+0.25*Z*((5.*QM(IZ+1)-3.0*QM(IZ)-QM(IZ-1)-QM(IZ+2))+(QM D   61
     1(IZ-1)-QM(IZ)-QM(IZ+1)+QM(IZ+2))*Z)                                D   62
   45 CONTINUE                                                           D   63
      IF (TNOW.NE.TEMP.AND.TNOW.GT.0.) FCT=((3355.7046E-6)*TNOW-1.)/TNOW D   64
   50 DO 70 IR=1,NR                                                      D   65
      I=KR(IR,1)                                                         D   66
      IF (I.EQ.0.OR.R(IR).EQ.0.) GO TO 70                                D   67
C                                                                        D   68
C     CHECK FOR A ZEROTH ORDER REACTION                                  D   69
C                                                                        D   70
      RT=1.                                                              D   71
      JT=ITYPE(IR)                                                       D   72
      DO 55 L=1,JT                                                       D   73
      I=KR(IR,L)                                                         D   74
      IF (I.EQ.99.OR.I.EQ.0) GO TO 55                                    D   75
      IF (I.NE.NS) RT=RT*X(I)                                            D   76
      IF (I.EQ.NS) RT=RT*P                                               D   77
   55 CONTINUE                                                           D   78
      IF (ABS(S(IR)).NE.0..AND.T.GT.1.) R(IR)=A(IR)*EXP(S(IR)*FCT)       D   79
      RT=RT*R(IR)                                                        D   80
      DO 60 L=1,JT                                                       D   81
      I=KR(IR,L)                                                         D   82
      IF (I.EQ.0.OR.I.GT.N) GO TO 60                                     D   83
      XT(I)=XT(I)-RT                                                     D   84
   60 CONTINUE                                                           D   85
      DO 65 K=4,7                                                        D   86
      I=KR(IR,K)                                                         D   87
      IF (I.EQ.0) GO TO 70                                               D   88
C                                                                        D   89
C     I WILL BE NEGATIVE IF CLEAN HAS BEEN CALLED                        D   90
C                                                                        D   91
      IF (I.LT.0) GO TO 65                                               D   92
      XT(I)=XT(I)+SC(IR,K)*RT                                            D   93
   65 CONTINUE                                                           D   94
   70 CONTINUE                                                           D   95
      TEMP=TNOW                                                          D   96
      TOLD=T                                                             D   97
      RETURN                                                             D   98
      END                                                                D   99-
```

```
      SUBROUTINE MATRX (C,KR)                                              E    1
C                                                                          E    2
C*************************************************************************** E    3
C                                                                          E    4
C     MATRX CREATES A NR X 7 MATRIX OF THE REACTION SCHEME WHERE EACH      E    5
C     ROW REPRESENTS A  REACTION.  THE FIRST THREE COLUMNS ARE REACTANTS   E    6
C     AND THE LAST FOUR ARE THE PRODUCTS.  THE ELEMENTS CORRESPOND         E    7
C     TO THE INDIVIDUAL SPECIES AND WILL BE USED AS SUBSCRIPTS.            E    8
C                                                                          E    9
C*************************************************************************** E   10
C                                                                          E   11
      INTEGER SPECIS,REACT                                                 E   12
      COMMON /DATA/ NR,IR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,   E   13
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT             E   14
      COMMON /NAMES/ SPECIS(91),REACT(91),NS                               E   15
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS1,UROUND,NC,MF1,KFLAG1,JSTART        E   16
      COMMON /ALPHA/ IGO(4),IBLANK,MBLANK,JINTER                           E   17
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP                   E   18
      DIMENSION C(91), KR(200,7)                                           E   19
      NOLD=NS+1                                                            E   20
      DO 90 I=1,NR                                                         E   21
C                                                                          E   22
C     SKIP REACTIONS ALREADY PROCESSED                                     E   23
C                                                                          E   24
      IF (IR(I,2).EQ.NOLD.OR.IR(I,3).EQ.NOLD) IR(I,3)=99                   E   25
      IF (IR(I,2).EQ.NOLD) IR(I,2)=0                                       E   26
      IF (IR(I,1).EQ.NOLD) IR(I,1)=99                                      E   27
      IF (IR(I,1).EQ.NOLD) IR(I,3)=99                                      E   28
      IF (IABS(IR(I,1)).NE.100) GO TO 90                                   E   29
C                                                                          E   30
C     IF LESS THAN THREE REACTANTS, FILL FIRST SLOTS.                      E   31
C                                                                          E   32
      IF (KR(I,1).NE.IBLANK) GO TO 5                                       E   33
      IF (KR(I,3).NE.IBLANK) KR(I,1)=KR(I,3)                               E   34
      IF (KR(I,3).NE.IBLANK) SC(I,1)=SC(I,3)                               E   35
      SC(I,3)=1.                                                           E   36
      KR(I,3)=IBLANK                                                       E   37
      IF (KR(I,1).NE.IBLANK) GO TO 5                                       E   38
      KR(I,1)=KR(I,2)                                                      E   39
      KR(I,2)=IBLANK                                                       E   40
      SC(I,1)=SC(I,2)                                                      E   41
      SC(I,2)=1.                                                           E   42
    5 IF (KR(I,2).NE.IBLANK) GO TO 10                                      E   43
      IF (KR(I,3).NE.IBLANK) SC(I,2)=SC(I,3)                               E   44
      SC(I,3)=1.                                                           E   45
      IF (KR(I,3).NE.IBLANK) KR(I,2)=KR(I,3)                               E   46
      KR(I,3)=IBLANK                                                       E   47
   10 DO 15 K=4,7                                                          E   48
C                                                                          E   49
C     GET RID OF M AS A PRODUCT                                            E   50
```

```
C                                                                       E   51
      IF (KR(I,K).EQ.MBLANK) KR(I,K)=IBLANK                             E   52
   15 CONTINUE                                                          E   53
C                                                                       E   54
C     IF LESS THAN FOUR PRODUCTS, FILL FIRST SLOTS.                     E   55
C                                                                       E   56
      IF (KR(I,4).NE.IBLANK) GO TO 30                                   E   57
      DO 20 K=1,3                                                       E   58
      INDEX=8-K                                                         E   59
      IF (KR(I,INDEX).NE.IBLANK) GO TO 25                               E   60
   20 CONTINUE                                                          E   61
      INDEX=5                                                           E   62
   25 KR(I,4)=KR(I,INDEX)                                               E   63
      KR(I,INDEX)=IBLANK                                                E   64
      SC(I,4)=SC(I,INDEX)                                               E   65
      SC(I,INDEX)=1.                                                    E   66
      IF (KR(I,1).NE.IBLANK.OR.KR(I,4).NE.IBLANK) GO TO 30              E   67
      IR(I,1)=0                                                         E   68
      GO TO 90                                                          E   69
   30 CONTINUE                                                          E   70
      IF (KR(I,5).NE.IBLANK) GO TO 35                                   E   71
      IF (KR(I,7).NE.IBLANK) KR(I,5)=KR(I,7)                            E   72
      IF (KR(I,7).NE.IBLANK) SC(I,5)=SC(I,7)                            E   73
      SC(I,7)=1.                                                        E   74
      KR(I,7)=IBLANK                                                    E   75
      IF (KR(I,5).NE.IBLANK) GO TO 35                                   E   76
      KR(I,5)=KR(I,6)                                                   E   77
      KR(I,6)=IBLANK                                                    E   78
      SC(I,5)=SC(I,6)                                                   E   79
      SC(I,6)=1.                                                        E   80
   35 K=KR(I,6)                                                         E   81
      IF (K.NE.IBLANK) GO TO 40                                         E   82
      KR(I,6)=KR(I,7)                                                   E   83
      KR(I,7)=K                                                         E   84
      SC(I,6)=SC(I,7)                                                   E   85
      SC(I,7)=1.                                                        E   86
   40 DO 85 J=1,7                                                       E   87
      K=KR(I,J)                                                         E   88
C                                                                       E   89
C     PROCESS REACTANTS HERE                                            E   90
C                                                                       E   91
      IF (J.GT.3) GO TO 65                                              E   92
C                                                                       E   93
C     ALL M DEPENDENT REACTIONS ARE TO HAVE A 99 IN THE THIRD SLOT      E   94
C                                                                       E   95
      IF (K.NE.MBLANK) GO TO 60                                         E   96
      GO TO (45,50,55),J                                                E   97
   45 KR(I,1)=KR(I,2)                                                   E   98
      SC(I,1)=SC(I,2)                                                   E   99
   50 KR(I,2)=KR(I,3)                                                   E  100
```

```
      SC(I,2)=SC(I,3)                                                    E  101
      SC(I,3)=1.                                                         E  102
      KR(I,3)=MBLANK                                                     E  103
   55 IR(I,3)=99                                                         E  104
   60 K=KR(I,J)                                                          E  105
C                                                                        E  106
C     ZERO ORDER REACTIONS HAVE 99 IN FIRST SLOT                         E  107
C                                                                        E  108
      IF (KR(I,1).EQ.IBLANK) IR(I,1)=99                                  E  109
      IF (KR(I,1).EQ.IBLANK) K=99                                        E  110
C                                                                        E  111
C     ALL BLANKS ARE SET EQUAL TO ZERO                                   E  112
C                                                                        E  113
      IF (J.EQ.3.AND.K.EQ.MBLANK) K=99                                   E  114
   65 IF (K.EQ.MBLANK.OR.K.EQ.IBLANK) IR(I,J)=0                          E  115
      IF (K.EQ.IBLANK.OR.K.EQ.99) GO TO 85                               E  116
      IF (NS.NE.0) GO TO 70                                              E  117
      NS=1                                                               E  118
      GO TO 80                                                           E  119
   70 DO 75 L=1,NS                                                       E  120
      IF (K.NE.SPECIS(L)) GO TO 75                                       E  121
C                                                                        E  122
C     SLOT SET TO SPECIES NUMBER                                         E  123
C                                                                        E  124
      IR(I,J)=L                                                          E  125
      GO TO 85                                                           E  126
   75 CONTINUE                                                           E  127
C                                                                        E  128
C     IF NO SPECIES ARE FOUND, ADD ONE TO THE LIST                       E  129
C                                                                        E  130
      IF (SPECIS(NS).NE.ITEMP) NS=NS+1                                   E  131
   80 SPECIS(NS)=K                                                       E  132
      C(NS+2)=C(NS+1)                                                    E  133
      C(NS+1)=C(NS)                                                      E  134
      C(NS)=0.                                                           E  135
      IR(I,J)=NS                                                         E  136
   85 CONTINUE                                                           E  137
   90 CONTINUE                                                           E  138
      IF (SPECIS(NS).NE.ITEMP) NS=NS+1                                   E  139
      SPECIS(NS)=ITEMP                                                   E  140
      SPECIS(NS+1)=MBLANK                                                E  141
      NS=NS+1                                                            E  142
      DO 95 IK=1,NR                                                      E  143
      DO 95 MT=1,3                                                       E  144
      J=IFIX(SC(IK,MT)+UROUND)                                           E  145
      ISC(IK,MT)=J                                                       E  146
   95 IF (SC(IK,MT)-FLOAT(J).GT.4.*UROUND) ISC(IK,MT)=-1                 E  147
      DO 100 I=1,NR                                                      E  148
      IF (IR(I,1).EQ.0) GO TO 100                                        E  149
      ITYPE(I)=2                                                         E  150
```

```
C                                                                       E  151
C     CHECK FOR 99 CODE AND SUBSTITUTE M WHICH IS THE LAST SPECIES      E  152
C                                                                       E  153
      IF (IR(I,1).EQ.99.AND.IR(I,3).EQ.99) IR(I,1)=NS                   E  154
      IF (IR(I,1).EQ.NS.AND.IR(I,3).EQ.99) IR(I,3)=0                    E  155
      IF (IR(I,2).EQ.0.AND.IR(I,3).EQ.99) IR(I,2)=NS                    E  156
      IF (IR(I,2).EQ.NS.AND.IR(I,3).EQ.99) IR(I,3)=0                    E  157
      IF (IR(I,2).EQ.0) ITYPE(I)=1                                      E  158
      IF (IR(I,3).NE.0) ITYPE(I)=3                                      E  159
      IF (IR(I,3).EQ.99) IR(I,3)=NS                                     E  160
  100 CONTINUE                                                          E  161
      RETURN                                                            E  162
      END                                                               E  163-
```

```
      SUBROUTINE PLOT (NTIT,NPNT,NTOT,NAME,SAVTIM,SAVCON,IDT,KCP,JGRID)  F    1
C SUBROUTINE ****** P L O T ******                                       F    2
C                                                                        F    3
C THIS SUBROUTINE READS THE PLOT CARDS AND PLOTS THE RESULTS AS PART     F    4
C OF THE PRINTED OUTPUT -- IT DOES NOT DRIVE A PLOTTER.                  F    5
C                                                                        F    6
C SYMBOL DESCRIPTIONS --                                                 F    7
C                                                                        F    8
C CGRID    THE LENGTH OF THE VERTICAL AXIS, PPM                          F    9
C CHIGH    HIGHEST CONCENTRATION VALUE, PPM                              F   10
C CLOW     LOWEST CONCENTRATION VALUE, PPM                               F   11
C CSPAN    CONCENTRATION NORMALIZATION FACTOR                            F   12
C DATA     CONCENTRATION DATA POINTS, PPM, UP TO 80                      F   13
C IDT      IF NOT ZERO THEN PRINT RAW DATA USED FOR PLOTS                F   14
C J        DO-LOOP INDICES OR LOCAL POINTERS                             F   15
C JBLANK   A HOLLERITH WORD OF FOUR BLANK CHARACTERS                     F   16
C JCONC    CONCENTRATION LABELS                                          F   17
C JGRID    THE PLOTTING GRID                                             F   18
C JN       HOLLERITH SYMBOL FOR NO DATA POINTS                           F   19
C JPLUS    THE CHARACTER >+>                                             F   20
C JSTAR    THE CHARACTER >*>                                             F   21
C JSYMB    SYMBOL TO BE USED FOR PLOTTING SAVED POINTS                   F   22
C JVERT    VERTICAL LEGEND                                               F   23
C JX       THE CHARACTER >X>                                             F   24
C K        DO-LOOP INDICES OR LOCAL POINTERS                             F   25
C KCP      IF NOT EQUAL TO ZERO SAVE DATA FOR OFFLINE PLOTTING           F   26
C KCON     CONCENTRATION COORDINATE ON GRID                              F   27
C KTIM     TIME COORDINATE ON GRID                                       F   28
C L        DO-LOOP INDICES OR LOCAL POINTERS                             F   29
C M        DO-LOOP INDICES OR LOCAL POINTERS                             F   30
C MAXCON   LIMIT ON NUMBER OF VERTICAL POINTS                            F   31
C MAXPNT   MAXIMUM NUMBER OF SAVED TIME AND CONCENTRATION POINTS         F   32
C MAXTIM   LIMIT ON NUMBER OF HORIZONTAL POINTS                          F   33
C N        DO-LOOP INDICES OR LOCAL POINTERS                             F   34
C NAME     SPECIES NAMES, ONE PER SPECIES                                F   35
C NDAT     NUMBER OF CONCENTRATION DATA POINTS                           F   36
C NIN      THE FORTRAN INPUT UNIT (NORMALLY 5)                           F   37
C NOUT     THE FORTRAN OUTPUT UNIT NUMBER (NORMALLY 6)                   F   38
C NPLT     THE NUMBER OF SPECIES TO BE PLOTTED                           F   39
C NPNT     NUMBER OF SAVED TIMES AND CONCENTRATIONS                      F   40
C NTEST    SPECIES NAME FOR TESTING                                      F   41
C NTIT     USER-INPUT TITLE FOR PRINTOUT, 3 FOUR-CHARACTER WORDS         F   42
C NTOT     TOTAL NUMBER OF SPECIES                                       F   43
C NX       FLAG FOR CORRECT SPECIES TEST                                 F   44
C SAVCON   SPECIES CONCENTRATIONS, PPM, ONE PER SPECIES AT 80 TIMES      F   45
C SAVTIM   TIMES THAT CONCENTRATIONS ARE SAVED, MIN, UP TO 80 VALUES     F   46
C TGRID    THE LENGTH OF THE HORIZONTAL AXIS, MIN                        F   47
C THIGH    HIGHEST TIME VALUE, MIN                                       F   48
C TIME     TIMES AT WHICH CONCENTRATIONS ARE INPUT, MIN, UP TO 80        F   49
C TLOW     LOWEST TIME VALUE, MIN                                        F   50
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C TPRINT   TIMES FOR PRINTOUT ON HORIZONTAL AXIS, MIN                    F   51
C TSPAN    TIME NORMALIZATION FACTOR                                     F   52
C                                                                        F   53
C BEGINNING OF PROGRAM.                                                  F   54
C                                                                        F   55
C ENTRY POINT                                                            F   56
C                                                                        F   57
C SET DIMENSIONS OF INCOMING ARRAYS                                      F   58
C                                                                        F   59
      DIMENSION SAVCON(90,80), SAVTIM(80), NTIT(3), NAME(91)             F   60
C                                                                        F   61
C SET DIMENSIONS OF LOCAL ARRAYS                                         F   62
C                                                                        F   63
      DIMENSION JCONC(5), TIME(80), DATA(80), JN(3)                      F   64
      DIMENSION JGRID(89,40), TPRINT(9), KVERT(52)                       F   65
C                                                                        F   66
C DEFINE THE VERTICAL LABEL AND ESTABLISH ALPHAMERIC DATA                F   67
C                                                                        F   68
      COMMON /APLOT/ JVERT(52,2),JBLANK,JSTAR,JPLUS,JBAR                 F   69
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10                      F   70
C                                                                        F   71
C DEFINE MISCELLANEOUS DATA VALUES                                       F   72
C                                                                        F   73
      COMMON /INOUT/ NIN,NOUT,ITAPE                                      F   74
      DATA MAXTIM/89/,MAXCON/40/,MAXPNT/80/                              F   75
      DATA TGRID/88./,CGRID/40./,JX/1HX/,JNO/1H /                        F   76
      DATA KVERT/11*4H     ,4H P  ,4H H  ,4H O  ,4H T  ,4H O  ,4H L  ,4H  F   77
     1Y  ,4H S  ,4H I  ,4H S  ,4H     ,4H C  ,4H O  ,4H N  ,4H S  ,4H T   F   78
     2,4H A  ,4H N  ,4H T  ,22*4H    /                                   F   79
C                                                                        F   80
C DEFINE VERTICAL AXIS VIA ASSIGNMENT STATEMENTS                         F   81
C                                                                        F   82
      IF (IDT*IDT.EQ.0) GO TO 10                                         F   83
      WRITE (NOUT,150)                                                   F   84
      WRITE (NOUT,145) (NAME(I),I=1,NTOT)                                F   85
      DO 5 J=1,NPNT                                                      F   86
    5 WRITE (NOUT,155) SAVTIM(J),(SAVCON(I,J),I=1,NTOT)                  F   87
   10 DO 15 J=1,40                                                       F   88
      JGRID(1,J)=JBAR                                                    F   89
   15 CONTINUE                                                           F   90
      JGRID(1,1)=JPLUS                                                   F   91
      JGRID(1,11)=JPLUS                                                  F   92
      JGRID(1,21)=JPLUS                                                  F   93
      JGRID(1,31)=JPLUS                                                  F   94
      JN(1)=JSTAR                                                        F   95
      JN(2)=JPLUS                                                        F   96
      JN(3)=JX                                                           F   97
      TSPAN=-10.                                                         F   98
C                                                                        F   99
C READ PLOT CONTROL CARD                                                 F  100
```

```
C                                                                       F  101
   20 READ (NIN,130) NPLT,JCONC,CLOW,CHIGH,TLOW,THIGH                   F  102
C                                                                       F  103
C TEST FOR END PLOTTING                                                 F  104
C                                                                       F  105
      IF (NPLT.EQ.0) GO TO 105                                          F  106
      WRITE (NOUT,160) NTIT                                             F  107
C                                                                       F  108
C SET NORMALIZATION FACTORS AND VERTICAL LABELS                         F  109
C                                                                       F  110
      CSPAN=CGRID/(CHIGH-CLOW)                                          F  111
      TSPAN=TGRID/(THIGH-TLOW)                                          F  112
      JVERT(1,2)=JCONC(5)                                               F  113
      JVERT(11,2)=JCONC(4)                                              F  114
      JVERT(21,2)=JCONC(3)                                              F  115
      JVERT(31,2)=JCONC(2)                                              F  116
C                                                                       F  117
C SET HORIZONTAL TIME LABELS                                            F  118
C                                                                       F  119
      DO 25 J=1,9                                                       F  120
      TPRINT(J)=FLOAT(J-1)/8.*(THIGH-TLOW)+TLOW                         F  121
   25 CONTINUE                                                          F  122
C                                                                       F  123
C CLEAR GRID                                                            F  124
C                                                                       F  125
      DO 35 K=1,MAXCON                                                  F  126
      DO 30 J=2,MAXTIM                                                  F  127
      JGRID(J,K)=JBLANK                                                 F  128
   30 CONTINUE                                                          F  129
   35 CONTINUE                                                          F  130
      NX=0                                                              F  131
      DO 95 LK=1,NPLT                                                   F  132
      READ (NIN,135) NTEST,NDAT,JSYMB                                   F  133
C                                                                       F  134
C TEST NUMBER OF DATA POINTS AND READ DATA                              F  135
C                                                                       F  136
      IF (NDAT.LE.0) GO TO 45                                           F  137
      IF (NDAT.LE.MAXPNT) GO TO 40                                      F  138
      WRITE (NOUT,185) MAXPNT                                           F  139
      GO TO 125                                                         F  140
C                                                                       F  141
C READ DATA POINTS                                                      F  142
C                                                                       F  143
   40 READ (NIN,140) (TIME(J),DATA(J),J=1,NDAT)                         F  144
C                                                                       F  145
C TEST FOR CORRECT SPECIES NAME                                         F  146
C                                                                       F  147
   45 DO 50 L=1,NTOT                                                    F  148
      IF (NTEST.EQ.NAME(L)) GO TO 55                                    F  149
   50 CONTINUE                                                          F  150
```

```
      WRITE (NOUT,190) NTEST                                              F 151
      NX=NX+1                                                             F 152
      IF (NPLT.EQ.1.OR.NX.EQ.3) GO TO 20                                  F 153
      IF (NPLT.EQ.2.AND.NX.EQ.2) GO TO 20                                 F 154
      GO TO 95                                                            F 155
C                                                                         F 156
C IF THERE ARE CALCULATED POINTS, GET THEIR COORDINATES                   F 157
C                                                                         F 158
   55 IF (NPNT.LE.0) GO TO 65                                             F 159
      DO 60 J=1,NPNT                                                      F 160
      KTIM=IFIX((SAVTIM(J)-TLOW)*TSPAN+1.5)                               F 161
      Y=(SAVCON(L,J)-CLOW)*CSPAN-0.5                                      F 162
      IF (Y.LT.0.0) GO TO 60                                              F 163
      KCON=IFIX(Y)                                                        F 164
      KCON=MAXCON-KCON                                                    F 165
C                                                                         F 166
C CHECK FOR BEING WITHIN GRID, THEN PLACE ON GRID                         F 167
C                                                                         F 168
      IF (KTIM.LT.2) GO TO 60                                             F 169
      IF (KCON.LT.1) GO TO 60                                             F 170
      IF (KTIM.GT.MAXTIM) GO TO 60                                        F 171
      IF (KCON.GT.MAXCON) GO TO 60                                        F 172
      JGRID(KTIM,KCON)=JSYMB                                              F 173
   60 CONTINUE                                                            F 174
C                                                                         F 175
C IF THERE ARE DATA POINTS, GET THEIR COORDINATES                         F 176
C                                                                         F 177
   65 IF (NDAT.LE.0) GO TO 75                                             F 178
      DO 70 J=1,NDAT                                                      F 179
      KTIM=IFIX((TIME(J)-TLOW)*TSPAN+1.5)                                 F 180
      Y=(DATA(J)-CLOW)*CSPAN-0.5                                          F 181
      IF (Y.LT.0.0) GO TO 70                                              F 182
      KCON=IFIX(Y)                                                        F 183
      KCON=MAXCON-KCON                                                    F 184
C                                                                         F 185
C CHECK FOR BEING WITHIN GRID, THEN PLACE ON GRID                         F 186
C                                                                         F 187
      IF (KTIM.LT.2) GO TO 70                                             F 188
      IF (KCON.LT.1) GO TO 70                                             F 189
      IF (KTIM.GT.MAXTIM) GO TO 70                                        F 190
      IF (KCON.GT.MAXCON) GO TO 70                                        F 191
      IF (LK.EQ.1) JGRID(KTIM,KCON)=JSTAR                                 F 192
      IF (LK.EQ.2) JGRID(KTIM,KCON)=JPLUS                                 F 193
      IF (LK.EQ.3) JGRID(KTIM,KCON)=JX                                    F 194
   70 CONTINUE                                                            F 195
   75 IF (NDAT.GT.0) GO TO 85                                             F 196
      WRITE (NOUT,195) NTEST,JNO,JSYMB                                    F 197
      GO TO 90                                                            F 198
   85 WRITE (NOUT,195) NTEST,JN(LK),JSYMB                                 F 199
C                                                                         F 200
```

```
C SAVE DATA FOR OFFLINE PLOTS IF DESIRED                                F  201
C                                                                       F  202
   90 IF (KCP*KCP.EQ.0) GO TO 95                                        F  203
      WRITE (ITAPE) NTIT,NAME(L),CLOW,CHIGH,TLOW,THIGH,NDAT,NPNT,(TIME(J F  204
     1),J=1,NDAT),(DATA(J),J=1,NDAT),(SAVTIM(J),J=1,NPNT),(SAVCON(L,J),J F  205
     2=1,NPNT)                                                          F  206
   95 CONTINUE                                                          F  207
      DO 100 K=1,MAXCON                                                 F  208
      WRITE (NOUT,165) JVERT(K,1),JVERT(K,2),(JGRID(J,K),J=1,MAXTIM)    F  209
  100 CONTINUE                                                          F  210
C                                                                       F  211
C PRINT THE HORIZONTAL AXIS AND LABELS                                  F  212
C                                                                       F  213
      WRITE (NOUT,170) JCONC(1)                                         F  214
      IF (THIGH.GT.80.) WRITE (NOUT,175) TPRINT                         F  215
      IF (THIGH.LE.80.) WRITE (NOUT,180) TPRINT                         F  216
      GO TO 20                                                          F  217
C                                                                       F  218
C END OF SUBROUTINE -- RETURN TO CALLER                                 F  219
C                                                                       F  220
  105 IF (IPP.LE.0) RETURN                                              F  221
      IF (IN10.LE.0) RETURN                                             F  222
      IF (TSPAN.LE.0.) RETURN                                           F  223
      JVERT(1,2)=4H0.80                                                 F  224
      JVERT(11,2)=4H0.60                                                F  225
      JVERT(21,2)=4H0.40                                                F  226
      JVERT(31,2)=4H0.20                                                F  227
      JCONC(1)=4H0.00                                                   F  228
      CSPAN=CGRID/0.8                                                   F  229
      WRITE (NOUT,200) NTIT                                             F  230
      DO 110 I=1,MAXCON                                                 F  231
      DO 110 J=2,MAXTIM                                                 F  232
  110 JGRID(J,I)=JBLANK                                                 F  233
      DO 115 I=1,NPNT                                                   F  234
      KTIM=IFIX((RTIM(I)-TLOW)*TSPAN+1.5)                               F  235
      Y=(RDAT(I)-CLOW)*CSPAN-0.5                                        F  236
      IF (Y.LT.0.0) GO TO 115                                           F  237
      KCON=IFIX(Y)                                                      F  238
      KCON=MAXCON-KCON                                                  F  239
      IF (KCON.LT.1) GO TO 115                                          F  240
      IF (KTIM.LT.2) GO TO 115                                          F  241
      IF (KTIM.GT.MAXTIM) GO TO 115                                     F  242
      IF (KCON.GT.MAXCON) GO TO 115                                     F  243
      JGRID(KTIM,KCON)=JSTAR                                            F  244
  115 CONTINUE                                                          F  245
      DO 120 K=1,MAXCON                                                 F  246
      WRITE (NOUT,165) KVERT(K),JVERT(K,2),(JGRID(J,K),J=1,MAXTIM)      F  247
  120 CONTINUE                                                          F  248
      WRITE (NOUT,170) JCONC(1)                                         F  249
      IF (TPRINT(9).GT.80.) WRITE (NOUT,175) TPRINT                     F  250
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```
      IF (TPRINT(9).LE.80.) WRITE (NOUT,180) TPRINT                    F  251
      RETURN                                                           F  252
  125 CONTINUE                                                         F  253
      STOP                                                             F  254
C                                                                      F  255
C LIST OF FORMAT STATEMENTS                                            F  256
C                                                                      F  257
C                                                                      F  258
C                                                                      F  259
  130 FORMAT (5X,I2,8X,5(A4,1X),4F10.0)                                F  260
  135 FORMAT (A4,1X,I2,1X,A1)                                          F  261
  140 FORMAT (8F10.0)                                                  F  262
  145 FORMAT (/,4X,5HTIME ,4X,10(4X,A4,4X),/,(13X,10(4X,A4,4X)))       F  263
  150 FORMAT (1H1)                                                     F  264
  155 FORMAT (1P11E12.4,/,(12X,10E12.4))                               F  265
  160 FORMAT (1H1,//////////,62X,3A4,/,32X,7HSPECIES,2X,5HEXPT.,2X,4HSIM F  266
     1.)                                                               F  267
  165 FORMAT (16X,2A4,89A1)                                            F  268
  170 FORMAT (20X,A4,1H+,8(11H----------+))                            F  269
  175 FORMAT (I25,2X,8F11.0,/,62X,14HTIME (MINUTES),/)                 F  270
  180 FORMAT (I25,2X,8F11.3,/,62X,14HTIME (MINUTES),/)                 F  271
  185 FORMAT (33H PROGRAM CANNOT HANDLE MORE THAN ,I4,28H PLOT POINTS -- F  272
     1 JOB ABORTED.)                                                   F  273
  190 FORMAT (33X,13HSPECIES NAME ,A4,26H NOT FOUND IN SPECIES LIST)   F  274
  195 FORMAT (33X,A4,6X,A1,5X,A1)                                      F  275
  200 FORMAT (1H1,//////////,62X,3A4,//)                               F  276
      END                                                              F  277-
```

```
      SUBROUTINE VALU (VAL,N,NF,NL)                                      G    1
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST, G    2
     1IPH(30),QM(100),PM(100),PSTOP                                      G    3
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS1,UROUND,NC,MF1,KFLAG1,JSTART      G    4
      DIMENSION AC(5), AD(5), BC(5)                                      G    5
      INTEGER AC,AD,BC,AST                                               G    6
      DATA IBLK/1H /,IPER/1H./,IZRO/1H0/                                 G    7
      AVAL=ALOG10(VAL)                                                   G    8
      IF (AVAL.EQ.0.) RETURN                                             G    9
      DO 5 I=1,5                                                         G   10
      AC(I)=IBLK                                                         G   11
      AD(I)=IZRO                                                         G   12
    5 BC(I)=IZRO                                                         G   13
      IAD=IFIX(AVAL+UROUND)                                              G   14
      IF (IAD) 30,10,10                                                  G   15
   10 IREM=3-IAD                                                         G   16
      IAD=IAD+1                                                          G   17
      JREM=IFIX(VAL+UROUND)                                              G   18
      REM=VAL-FLOAT(JREM)                                                G   19
      IF (REM.GT.UROUND.AND.IREM.GT.0) GO TO 15                          G   20
      CALL CONVT (JREM,AC,5)                                             G   21
      GO TO 50                                                           G   22
   15 CALL CONVT (JREM,AD,IAD)                                           G   23
      JREM=IFIX(REM*(10.**IREM)+0.1)                                     G   24
      CALL CONVT (JREM,BC,IREM)                                          G   25
      DO 20 J=1,IAD                                                      G   26
   20 AC(J)=AD(J)                                                        G   27
      AC(IAD+1)=IPER                                                     G   28
      DO 25 K=1,IREM                                                     G   29
   25 AC(K+IAD+1)=BC(K)                                                  G   30
      GO TO 40                                                           G   31
   30 IAD=IABS(IFIX(AVAL-0.1))-1                                         G   32
      IVAL=IFIX(VAL*10000.+0.1)                                          G   33
      CALL CONVT (IVAL,AC,5)                                             G   34
      AC(1)=IPER                                                         G   35
      DO 35 I=1,IAD                                                      G   36
   35 AC(I+1)=IZRO                                                       G   37
   40 IF (AC(5).NE.IZRO) GO TO 50                                        G   38
      DO 45 K=1,4                                                        G   39
      L=6-K                                                              G   40
   45 AC(L)=AC(L-1)                                                      G   41
      AC(1)=IBLK                                                         G   42
      GO TO 40                                                           G   43
   50 DO 55 I=NF,NL                                                      G   44
      K=I-NF+1                                                           G   45
   55 AST(I)=AC(K)                                                       G   46
      RETURN                                                             G   47
      END                                                                G   48-
```

```
      SUBROUTINE CONVT (NUM,L,N)                                        H    1
C                                                                       H    2
C  SUBROUTINE CONVT CONVERTS INTEGERS TO ALPHANUMERICS                  H    3
C     FOR PRINTING                                                      H    4
C                                                                       H    5
C  ASSUMES VALUE OF INTEGER IS POSITIVE                                 H    6
C                                                                       H    7
      DIMENSION L(5), JDIGIT(10)                                        H    8
C                                                                       H    9
      DATA JDIGIT/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/              H   10
      DATA JBLANK/1H /                                                  H   11
C                                                                       H   12
      NI=NUM                                                            H   13
      DO 5 I=1,N                                                        H   14
      L(I)=JBLANK                                                       H   15
    5 CONTINUE                                                          H   16
C                                                                       H   17
      DO 10 K=1,N                                                       H   18
      I=N-K+1                                                           H   19
      NEXT=NI/10                                                        H   20
      NDX=(NI-NEXT*10)+1                                                H   21
      L(I)=JDIGIT(NDX)                                                  H   22
      IF (NEXT.LE.0) GO TO 15                                           H   23
      NI=NEXT                                                           H   24
   10 CONTINUE                                                          H   25
C                                                                       H   26
   15 RETURN                                                            H   27
      END                                                               H   28-
```

```
      SUBROUTINE SAVLIN (T,C,N)                                          I    1
      COMMON /FRPLOT/ NIT(3),SAVCON(90,80),SAVTIM(80),JGRID(89,40),NT    I    2
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10                      I    3
      DIMENSION C(91)                                                    I    4
      DATA NFRST/1/                                                      I    5
      IF (NFRST.EQ.1) GO TO 5                                            I    6
      IF (T.EQ.TOLD) RETURN                                              I    7
    5 IF (NT.LT.0) RETURN                                                I    8
      NFRST=2                                                            I    9
      TOLD=T                                                             I   10
      IF (NT.GT.80) RETURN                                               I   11
      IF (T.LT.SAVTIM(NT)) RETURN                                        I   12
      SAVTIM(NT)=T                                                       I   13
      RTIM(NT)=T                                                         I   14
      DO 10 I=1,N                                                        I   15
   10 SAVCON(I,NT)=C(I)                                                  I   16
      RDAT(NT)=RR1                                                       I   17
      NT=NT+1                                                            I   18
      RETURN                                                             I   19
      END                                                                I   20-
```

```
      SUBROUTINE SPLNA (N,X,Y,J,D,C,W)                                  J    1
      DIMENSION X(10), Y(10), D(2), C(30), W(30)                        J    2
C     ------------------------------------------------------------------ J    3
C            OVER THE INTERVAL X(I) TO X(I+1), THE INTERPOLATING        J    4
C            POLYNOMIAL                                                 J    5
C                 Y=Y(I)+A(I)*Z+B(I)*Z**2+E(I)*Z**3                     J    6
C            WHERE Z=(X-X(I))/(X(I+1)-X(I))                             J    7
C            IS USED. THE COEFFICIENTS A(I),B(I) AND E(I) ARE COMPUTED  J    8
C            BY SPLNA AND STORED IN LOCATIONS C(3*I-2),C(3*I-1) AND     J    9
C            C(3*I) RESPECTIVELY.                                       J   10
C            WHILE WORKING IN THE ITH INTERVAL,THE VARIABLE Q WILL      J   11
C            REPRESENT Q=X(I+1) - X(I), AND Y(I) WILL REPRESENT         J   12
C            Y(I+1)-Y(I)                                                J   13
C     ------------------------------------------------------------------ J   14
C                                                                       J   15
      Q=X(2)-X(1)                                                       J   16
      YI=Y(2)-Y(1)                                                      J   17
      IF (J.EQ.2) GO TO 5                                               J   18
C     ------------------------------------------------------------------ J   19
C            IF THE FIRST DERIVATIVE AT THE END POINTS IS GIVEN,        J   20
C            A(1) IS KNOWN, AND THE SECOND EQUATION BECOMES             J   21
C            MERELY B(1)+E(1)=YI - Q*D(1).                              J   22
C     ------------------------------------------------------------------ J   23
      C(1)=Q*D(1)                                                       J   24
      C(2)=1.0                                                          J   25
      W(2)=YI-C(1)                                                      J   26
      GO TO 10                                                          J   27
C     ------------------------------------------------------------------ J   28
C            IF THE SECOND DERIVATIVE AT THE END POINTS IS GIVEN        J   29
C            B(1) IS KNOWN, THE SECOND EQUATION BECOMES                 J   30
C            A(1)+E(1)=YI-0.5*Q*Q*D(1). DURING THE SOLUTION OF          J   31
C            THE 3N-4 EQUATIONS,A1 WILL BE KEPT IN CELL C(2)            J   32
C            INSTEAD OF C(1) TO RETAIN THE TRIDIAGONAL FORM OF THE      J   33
C            COEFFICIENT MATRIX.                                        J   34
C     ------------------------------------------------------------------ J   35
    5 C(2)=0.0                                                          J   36
      W(2)=0.5*Q*Q*D(1)                                                 J   37
   10 M=N-2                                                             J   38
      IF (M.LE.0) GO TO 20                                              J   39
C     ------------------------------------------------------------------ J   40
C            UPPER TRIANGULARIZATION OF THE TRIDIAGONAL SYSTEM OF       J   41
C            EQUATIONS FOR THE COEFFICIENT MATRIX FOLLOWS--             J   42
C     ------------------------------------------------------------------ J   43
      DO 15 I=1,M                                                       J   44
      AI=Q                                                              J   45
      Q=X(I+2)-X(I+1)                                                   J   46
      H=AI/Q                                                            J   47
      C(3*I)=-H/(2.0-C(3*I-1))                                          J   48
      W(3*I)=(-YI-W(3*I-1))/(2.0-C(3*I-1))                              J   49
      C(3*I+1)=-H*H/(H-C(3*I))                                          J   50
```

```
      W(3*I+1)=(YI-W(3*I))/(H-C(3*I))                                    J  51
      YI=Y(I+2)-Y(I+1)                                                   J  52
      C(3*I+2)=1.0/(1.0-C(3*I+1))                                        J  53
   15 W(3*I+2)=(YI-W(3*I+1))/(1.0-C(3*I+1))                              J  54
C     ------------------------------------------------------------------ J  55
C           E(N-1) IS DETERMINED DIRECTLY FROM THE LAST EQUATION         J  56
C           OBTAINED ABOVE, AND THE FIRST OR SECOND DERIVATIVE           J  57
C           VALUE GIVEN AT THE END POINT.                                J  58
C     ------------------------------------------------------------------ J  59
   20 IF (J.EQ.1) GO TO 25                                               J  60
      C(3*N-3)=(Q*Q*D(2)/2.0-W(3*N-4))/(3.0-C(3*N-4))                    J  61
      GO TO 30                                                           J  62
   25 C(3*N-3)=(Q*D(2)-YI-W(3*N-4))/(2.0-C(3*N-4))                       J  63
   30 M=3*N-6                                                            J  64
      IF (M.LE.0) GO TO 40                                               J  65
C     ------------------------------------------------------------------ J  66
C           BACK SOLUTION FOR ALL COEFFICENTS EXCEPT                     J  67
C           A(1) AND B(1) FOLLOWS--                                      J  68
C     ------------------------------------------------------------------ J  69
      DO 35 II=1,M                                                       J  70
      I=M-II+3                                                           J  71
   35 C(I)=W(I)-C(I)*C(I+1)                                              J  72
   40 IF (J.EQ.1) GO TO 45                                               J  73
C     ------------------------------------------------------------------ J  74
C           IF THE SECOND DERIVATIVE IS GIVEN AT THE END POINTS,         J  75
C           A(1) CAN NOW BE COMPUTED FROM THE KNOWN VALUES OF            J  76
C           B(1) AND E(1). THEN A(1) AND B(1) ARE PUT INTO THEIR         J  77
C           PROPER PLACES IN THE C ARRAY.                                J  78
C     ------------------------------------------------------------------ J  79
      C(1)=Y(2)-Y(1)-W(2)-C(3)                                           J  80
      C(2)=W(2)                                                          J  81
      RETURN                                                             J  82
   45 C(2)=W(2)-C(3)                                                     J  83
      RETURN                                                             J  84
      END                                                                J  85-
```

```
      SUBROUTINE DRIVES (N,TO,HO,YO,TOUT,EPS,MF,INDEX,IA,JA)                K    1
      DIMENSION IA(1), JA(1), YO(N)                                         K    2
      DIMENSION Y(91,6)                                                     K    3
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART          K    4
      COMMON /GEAR2/ YMAX(100)/GEAR3/ERROR(100)/GEAR4/W1(90,3)              K    5
      COMMON /GEAR5/ IW1(91,9)/GEAR6/W2(2000)/GEAR7/IW2(2000)               K    6
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP                K    7
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,NZA,NPL,NPU,NZL,NZU,NZRO    K    8
      COMMON /INOUT/ INP,LOUT,ITAPE                                         K    9
      DATA NMX/90/,LENW2/2000/,LENIW2/2000/                                 K   10
      NGP=0                                                                 K   11
      IF (INDEX.EQ.4) GO TO 15                                              K   12
      IF (INDEX.EQ.0) GO TO 30                                              K   13
      IF (INDEX.EQ.2) GO TO 35                                              K   14
      IF (INDEX.EQ.-1) GO TO 40                                             K   15
      IF (INDEX.EQ.3) GO TO 45                                              K   16
      IF (INDEX.NE.1) GO TO 135                                             K   17
      IF (EPS.LE.0.) GO TO 120                                              K   18
      IF (N.LE.0) GO TO 125                                                 K   19
      IF ((TO-TOUT)*HO.GE.0.) GO TO 130                                     K   20
      MITER=MF-10*(MF/10)                                                   K   21
      IF ((MITER.NE.1).AND.(MITER.NE.2)) GO TO 15                           K   22
      NP1=N+1                                                               K   23
      NZA=IA(NP1)-1                                                         K   24
      MAX=LENIW2/2                                                          K   25
      IPTI2=MAX+1                                                           K   26
      CALL SORDER (N,IA,JA,IW1,IW1(1,5),MAX,IW2,IW2(IPTI2),IER)             K   27
      IPTI2=NZA+1                                                           K   28
      IF (IPTI2+NZA-1.GT.LENIW2) GO TO 145                                  K   29
      DO 5 I=1,NP1                                                          K   30
    5 IW1(I,2)=IA(I)                                                        K   31
      DO 10 I=1,NZA                                                         K   32
   10 IW2(I)=JA(I)                                                          K   33
      CALL NSCORD (N,IW1(1,2),IW2,IW1(1,3),IW2(IPTI2),IW1,IW1(1,5),IW1(1    K   34
     1,8))                                                                  K   35
      MAXPL=(LENIW2-NZA)/2                                                  K   36
      IPTI3=IPTI2+MAXPL                                                     K   37
      MAXPU=LENIW2-IPTI3+1                                                  K   38
      CALL NSSFAC (N,IW1(1,2),IW2,MAXPL,IW1(1,3),IW2(IPTI2),IW1(1,4),MAX    K   39
     1PU,IW1(1,5),IW2(IPTI3),IW1(1,6),Y(1,6),IW1(1,9),Y,Y(1,2),Y(1,3),IW    K   40
     21(1,7),IW1(1,8),Y(1,4),Y(1,5),IER)                                    K   41
      NPL=IW1(N,4)                                                          K   42
      NPU=IW1(N,6)                                                          K   43
      NZL=IW1(N+1,3)                                                        K   44
      NZU=IW1(N+1,5)                                                        K   45
      IPTR2=NZA+1                                                           K   46
      IPTR3=IPTR2+MAXO(NZA,NZL)                                             K   47
      IF (IPTR3+MAXO(NZA,NZU)-1.GT.LENW2) GO TO 145                         K   48
   15 DO 20 I=1,N                                                           K   49
      YMAX(I)=ABS(YO(I))                                                    K   50
```

```
      IF (YMAX(I).EQ.0.) YMAX(I)=1.E-10                                 K   51
   20 Y(I,1)=YO(I)                                                      K   52
      NC=N                                                              K   53
      T=TO                                                              K   54
      H=HO                                                              K   55
      NZRO=0                                                            K   56
      TST=EPS*1.E-10                                                    K   57
      DO 25 I=1,N                                                       K   58
   25 IF (Y(I,1).GT.TST) NZRO=NZRO+1                                    K   59
      NZRO=MAXO(NZRO,1)                                                 K   60
      NOLD=NZRO                                                         K   61
      HMIN=ABS(HO)                                                      K   62
      HMAX=ABS(TO-TOUT)*10.                                             K   63
      HMAX=AMIN1(HMAX,20.)                                              K   64
      EPSC=EPS                                                          K   65
      MFC=MF                                                            K   66
      JSTART=0                                                          K   67
      NO=N                                                              K   68
      NMX1=NMX+1                                                        K   69
      EPSJ=SQRT(UROUND)                                                 K   70
      NHCUT=0                                                           K   71
      GO TO 50                                                          K   72
   30 HMAX=ABS(TOUT-TOUTP)*10.                                          K   73
      HMAX=AMIN1(HMAX,20.)                                              K   74
      GO TO 80                                                          K   75
   35 HMAX=ABS(TOUT-TOUTP)*10.                                          K   76
      HMAX=AMIN1(HMAX,20.)                                              K   77
      IF ((T-TOUT)*H.GE.0.) GO TO 150                                   K   78
      GO TO 85                                                          K   79
   40 IF ((T-TOUT)*H.GE.0.) GO TO 140                                   K   80
      JSTART=-1                                                         K   81
      NC=N                                                              K   82
      EPSC=EPS                                                          K   83
      MFC=MF                                                            K   84
   45 CONTINUE                                                          K   85
   50 CALL STIFFS (Y,NO,IA,JA,W1,NMX,IW1,NMX1)                          K   86
      KGO=1-KFLAG                                                       K   87
      GO TO (55,95,110,100),KGO                                         K   88
   55 CONTINUE                                                          K   89
      D=0.                                                              K   90
      NZRO=0                                                            K   91
      DO 70 I=1,NC                                                      K   92
      IF (Y(I,1).GE.0.) GO TO 65                                        K   93
      NGP=NGP+1                                                         K   94
      DO 60 J=1,6                                                       K   95
      K=(J-1)*N+I                                                       K   96
   60 Y(K,1)=0.                                                         K   97
   65 CONTINUE                                                          K   98
      IF (Y(I,1).GT.TST) NZRO=NZRO+1                                    K   99
      AYI=ABS(Y(I,1))                                                   K  100
```

```
      YMAX(I)=AMAX1(1.E-10,AYI)                                    K  101
   70 D=D+(AYI/YMAX(I))**2                                         K  102
      NZRO=MAXO(NZRO,1)                                            K  103
      IF (NZRO.NE.NOLD) JSTART=-1                                  K  104
      D=D*(UROUND/EPS)**2                                          K  105
      DO 75 II=1,NC                                                K  106
   75 YO(II)=Y(II,1)                                               K  107
      CALL SAVLIN (T,YO,N)                                         K  108
      IF (D.GT.FLOAT(N)) GO TO 115                                 K  109
      IF (INDEX.EQ.3) GO TO 150                                    K  110
      IF (INDEX.EQ.2) GO TO 85                                     K  111
   80 IF ((T-TOUT)*H.LT.0.) GO TO 45                               K  112
      CALL INTERP (TOUT,Y,NO,YO)                                   K  113
      GO TO 160                                                    K  114
   85 IF (T.GE.TOUT) GO TO 90                                      K  115
      IF (((T+H)-TOUT).LE.0.) GO TO 45                             K  116
      H=(TOUT-T)*(1.+4.*UROUND)                                    K  117
      JSTART=-1                                                    K  118
      GO TO 45                                                     K  119
   90 JSTART=-1                                                    K  120
      H=AMIN1(H,1.)                                                K  121
      GO TO 150                                                    K  122
   95 CONTINUE                                                     K  123
  100 IF (NHCUT.EQ.10) GO TO 105                                   K  124
      NHCUT=NHCUT+1                                                K  125
      HMIN=.1*HMIN                                                 K  126
      H=.1*H                                                       K  127
      JSTART=-1                                                    K  128
      GO TO 45                                                     K  129
  105 WRITE (LOUT,165)                                             K  130
      IF (KGO.EQ.4) WRITE (LOUT,180) T                             K  131
      STOP                                                         K  132
  110 WRITE (LOUT,170) T,H                                         K  133
      STOP                                                         K  134
  115 WRITE (LOUT,175) T                                           K  135
      KFLAG=-2                                                     K  136
      STOP                                                         K  137
  120 WRITE (LOUT,185)                                             K  138
      STOP                                                         K  139
  125 WRITE (LOUT,190)                                             K  140
      STOP                                                         K  141
  130 WRITE (LOUT,195)                                             K  142
      STOP                                                         K  143
  135 WRITE (LOUT,200) INDEX                                       K  144
      STOP                                                         K  145
  140 WRITE (LOUT,205) T,TOUT,H                                    K  146
      STOP                                                         K  147
  145 WRITE (LOUT,210)                                             K  148
      STOP                                                         K  149
  150 TOUT=T                                                       K  150
```

```
      DO 155 I=1,N                                                      K  151
  155 YO(I)=Y(I,1)                                                      K  152
      CALL SAVLIN (TOUT,YO,N)                                           K  153
  160 INDEX=KFLAG                                                       K  154
      TOUTP=TOUT                                                        K  155
      HO=HUSED                                                          K  156
      IF (KFLAG.NE.0) HO=H                                              K  157
      RETURN                                                            K  158
C                                                                       K  159
C                                                                       K  160
  165 FORMAT (//44H PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT//)      K  161
  170 FORMAT (//35H KFLAG = -2 FROM INTEGRATOR AT T = ,E16.8,5H  H =,E16 K  162
     1.8/52H  THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED//)     K  163
  175 FORMAT (//37H INTEGRATION HALTED BY DRIVER AT T = ,E16.8/56H  EPS  K  164
     1TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION/)              K  165
  180 FORMAT (//35H KFLAG = -3 FROM INTEGRATOR AT T = ,E16.8/45H  CORREC K  166
     1TOR CONVERGENCE COULD NOT BE ACHIEVED/)                           K  167
  185 FORMAT (//28H ILLEGAL INPUT.. EPS .LE. 0.//)                      K  168
  190 FORMAT (//25H ILLEGAL INPUT.. N .LE. 0//)                         K  169
  195 FORMAT (//36H ILLEGAL INPUT.. (TO-TOUT)*H .GE. 0.//)              K  170
  200 FORMAT (//24H ILLEGAL INPUT.. INDEX =,I5//)                       K  171
  205 FORMAT (//44H INDEX = -1 ON INPUT WITH (T-TOUT)*H .GE. 0./4H T =,E K  172
     116.8,9H   TOUT =,E16.8,6H   H =,E15.8)                           K  173
  210 FORMAT (//42H INSUFFICIENT WORKING STORAGE IN IW2 OR W2//)        K  174
      END                                                               K  175-
```

```
      SUBROUTINE STIFFS (Y,NO,IA,JA,W1,NMX,IW1,NMX1)                    L    1
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS,UROUND,N,MF,KFLAG,JSTART         L    2
      COMMON /GEAR2/ YMAX(100)/GEAR3/ERROR(100)                         L    3
      COMMON /GEAR6/ W2(2000)/GEAR7/IW2(2000)                           L    4
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP            L    5
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,IDUMMY(5),NZRO          L    6
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START, L    7
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT          L    8
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP                L    9
      DIMENSION Y(NO,1), IA(1), JA(1), W1(NMX,1), IW1(NMX1,1)           L   10
      DIMENSION EL(13), TQ(4), RT(3)                                    L   11
      DATA EL(2)/1./,OLDLO/1./                                          L   12
      KFLAG=0                                                           L   13
      TOLD=T                                                            L   14
      IF (JSTART.GT.0) GO TO 50                                         L   15
      IF (JSTART.NE.0) GO TO 10                                         L   16
      CALL DIFFUN (N,T,Y,W1)                                            L   17
      DO 5 I=1,N                                                        L   18
    5 Y(I,2)=H*W1(I,1)                                                  L   19
      METH=MF/10                                                        L   20
      MITER=MF-10*METH                                                  L   21
      NQ=1                                                              L   22
      L=2                                                               L   23
      IDOUB=3                                                           L   24
      RMAX=1.E4                                                         L   25
      RC=0.                                                             L   26
      CRATE=1.                                                          L   27
      HOLD=H                                                            L   28
      MFOLD=MF                                                          L   29
      NSTEP=0                                                           L   30
      NSTEPJ=0                                                          L   31
      NFE=1                                                             L   32
      NJE=0                                                             L   33
      IRET=3                                                            L   34
      GO TO 15                                                          L   35
   10 IF (MF.EQ.MFOLD) GO TO 25                                         L   36
      MEO=METH                                                          L   37
      MIO=MITER                                                         L   38
      METH=MF/10                                                        L   39
      MITER=MF-10*METH                                                  L   40
      MFOLD=MF                                                          L   41
      IF (MITER.NE.MIO) IWEVAL=MITER                                    L   42
      IF (METH.EQ.MEO) GO TO 25                                         L   43
      IDOUB=L+1                                                         L   44
      IRET=1                                                            L   45
   15 CALL COSET (METH,NQ,EL,TQ,MAXDER)                                 L   46
      LMAX=MAXDER+1                                                     L   47
      RC=RC*EL(1)/OLDLO                                                 L   48
      OLDLO=EL(1)                                                       L   49
   20 FN=FLOAT(NZRO)                                                    L   50
```

```
      EDN=FN*(TQ(1)*EPS)**2                                          L   51
      E=FN*(TQ(2)*EPS)**2                                            L   52
      EUP=FN*(TQ(3)*EPS)**2                                          L   53
      BND=FN*(TQ(4)*EPS)**2                                          L   54
      EPSOLD=EPS                                                     L   55
      NOLD=NZRO                                                      L   56
      GO TO (30,35,50),IRET                                          L   57
   25 IF (EPS.EQ.EPSOLD.AND.NZRO.EQ.NOLD) GO TO 30                   L   58
      IRET=1                                                         L   59
      GO TO 20                                                       L   60
   30 IF (H.EQ.HOLD) GO TO 50                                        L   61
      RH=H/HOLD                                                      L   62
      H=HOLD                                                         L   63
      IREDO=3                                                        L   64
      GO TO 40                                                       L   65
   35 RH=AMAX1(RH,HMIN/ABS(H))                                       L   66
   40 RH=AMIN1(RH,HMAX/ABS(H),RMAX)                                  L   67
      R1=1.                                                          L   68
      DO 45 J=2,L                                                    L   69
      R1=R1*RH                                                       L   70
      DO 45 I=1,N                                                    L   71
   45 Y(I,J)=Y(I,J)*R1                                               L   72
      H=H*RH                                                         L   73
      RC=RC*RH                                                       L   74
      IDOUB=L+1                                                      L   75
      IF (IREDO.EQ.0) GO TO 290                                      L   76
   50 IF (ABS(RC-1.).GT.0.3) IWEVAL=MITER                            L   77
      IF (NSTEP.GE.NSTEPJ+20) IWEVAL=MITER                           L   78
      T=T+H                                                          L   79
      DO 55 J1=1,NQ                                                  L   80
      DO 55 J2=J1,NQ                                                 L   81
      J=(NQ+J1)-J2                                                   L   82
      DO 55 I=1,N                                                    L   83
   55 Y(I,J)=Y(I,J)+Y(I,J+1)                                         L   84
   60 DO 65 I=1,N                                                    L   85
   65 ERROR(I)=0.                                                    L   86
      M=0                                                            L   87
      CALL DIFFUN (N,T,Y,W1(1,2))                                    L   88
      NFE=NFE+1                                                      L   89
      IF (IWEVAL.LE.0) GO TO 140                                     L   90
      IWEVAL=0                                                       L   91
      RC=1.                                                          L   92
      NJE=NJE+1                                                      L   93
      NSTEPJ=NSTEP                                                   L   94
      CON=-H*EL(1)                                                   L   95
      ISV=M                                                          L   96
      LSV=L                                                          L   97
      NZ=IA(N+1)-1                                                   L   98
      DO 70 I=1,NZ                                                   L   99
   70 W2(I)=0.                                                       L  100
```

```
      DO 125 IR=1,NR                                                    L  101
      IF (KR(IR,1).EQ.0.OR.KR(IR,1).EQ.99) GO TO 125                    L  102
      MT=ITYPE(IR)                                                      L  103
      DO 85 I=1,MT                                                      L  104
      IF (KR(IR,I).EQ.N+2) GO TO 85                                     L  105
      JX=I+1-I/3*3                                                      L  106
      KX=I+2-I/2*3                                                      L  107
      J=KR(IR,JX)                                                       L  108
      K=KR(IR,KX)                                                       L  109
      XJ=1.                                                             L  110
      IF (J.EQ.0) GO TO 75                                              L  111
      XJ=Y(J,1)                                                         L  112
      IF (J.EQ.N+2) XJ=SG                                               L  113
   75 XK=1.                                                             L  114
      IF (K.EQ.0) GO TO 80                                              L  115
      XK=Y(K,1)                                                         L  116
      IF (K.EQ.N+2) XK=SG                                               L  117
   80 RT(I)=R(IR)*XJ*XK                                                 L  118
   85 CONTINUE                                                          L  119
      DO 120 K=1,MT                                                     L  120
      I=KR(IR,K)                                                        L  121
      IF (I.EQ.N+2) GO TO 120                                           L  122
      DO 100 L=1,MT                                                     L  123
      J=KR(IR,L)                                                        L  124
      IF (J.EQ.N+2) GO TO 100                                           L  125
      M=IA(J)-1                                                         L  126
   90 M=M+1                                                             L  127
      IF (I-JA(M)) 90,95,90                                             L  128
   95 W2(M)=W2(M)-RT(L)                                                 L  129
  100 CONTINUE                                                          L  130
      DO 115 L=4,7                                                      L  131
      J=KR(IR,L)                                                        L  132
      M=IA(I)-1                                                         L  133
      IF (J) 115,120,105                                                L  134
  105 M=M+1                                                             L  135
      IF (J-JA(M)) 105,110,105                                          L  136
  110 W2(M)=W2(M)+RT(K)*SC(IR,L)                                        L  137
  115 CONTINUE                                                          L  138
  120 CONTINUE                                                          L  139
  125 CONTINUE                                                          L  140
      DO 135 J=1,N                                                      L  141
      KMIN=IA(J)                                                        L  142
      KMAX=IA(J+1)-1                                                    L  143
      DO 130 K=KMIN,KMAX                                                L  144
      W2(K)=W2(K)*CON                                                   L  145
      IF (JA(K).EQ.J) W2(K)=W2(K)+1.-CON*DILUT                          L  146
  130 CONTINUE                                                          L  147
  135 CONTINUE                                                          L  148
      CALL NSCORA (N,IA,JA,W2,IW1(1,2),W2(IPTR3),W2(IPTR2),IW1,IW1(1,7), L  149
     1IW1(1,8))                                                         L  150
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```
      CALL NSNFAC (N,IW1(1,2),IW2,W2,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPT L  151
     1R2),W1(1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1,IW1(1,7),IW1 L  152
     2(1,8),IER)                                                         L  153
      M=ISV                                                              L  154
      L=LSV                                                              L  155
      IF (IER.NE.0) GO TO 160                                            L  156
  140 DO 145 I=1,N                                                       L  157
      IF (M.LE.0) GO TO 145                                              L  158
      IF (-H*W1(I,2)*10..GT.Y(I,1)) GO TO 155                            L  159
  145 W1(I,1)=H*W1(I,2)-(Y(I,2)+ERROR(I))                                L  160
      CALL NSBSLV (N,IW1,IW1,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPTR2),W1(1 L  161
     1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1(1,2),W1,W2)          L  162
      D=0.                                                               L  163
      DO 150 I=1,N                                                       L  164
      ERROR(I)=ERROR(I)+W1(I,2)                                          L  165
      D=D+(W1(I,2)/YMAX(I))**2                                           L  166
  150 W1(I,1)=Y(I,1)+EL(1)*ERROR(I)                                      L  167
      IF (M.NE.0) CRATE=AMAX1(.9*CRATE,D/D1)                             L  168
      IF ((D*AMIN1(1.,2.*CRATE)).LE.BND) GO TO 175                       L  169
      D1=D                                                               L  170
      M=M+1                                                              L  171
      IF (M.EQ.3) GO TO 155                                              L  172
      CALL DIFFUN (N,T,W1,W1(1,2))                                       L  173
      GO TO 140                                                          L  174
  155 NFE=NFE+2                                                          L  175
      IF (IWEVAL.EQ.-1) GO TO 170                                        L  176
  160 T=TOLD                                                             L  177
      RMAX=2.                                                            L  178
      DO 165 J1=1,NQ                                                     L  179
      DO 165 J2=J1,NQ                                                    L  180
      J=(NQ+J1)-J2                                                       L  181
      DO 165 I=1,N                                                       L  182
  165 Y(I,J)=Y(I,J)-Y(I,J+1)                                             L  183
      IF (ABS(H).LE.HMIN*1.00001) GO TO 285                              L  184
      RH=.25                                                             L  185
      IREDO=1                                                            L  186
      GO TO 35                                                           L  187
  170 IWEVAL=MITER                                                       L  188
      GO TO 60                                                           L  189
  175 IF (MITER.NE.0) IWEVAL=-1                                          L  190
      NFE=NFE+M                                                          L  191
      D=0.                                                               L  192
      DO 180 I=1,N                                                       L  193
  180 D=D+(ERROR(I)/YMAX(I))**2                                          L  194
      IF (D.GT.E) GO TO 195                                              L  195
      KFLAG=0                                                            L  196
      IREDO=0                                                            L  197
      NSTEP=NSTEP+1                                                      L  198
      HUSED=H                                                            L  199
      NQUSED=NQ                                                          L  200
```

```
      DO 185 J=1,L                                                    L  201
      DO 185 I=1,N                                                    L  202
  185 Y(I,J)=Y(I,J)+EL(J)*ERROR(I)                                    L  203
      IF (IDOUB.EQ.1) GO TO 205                                       L  204
      IDOUB=IDOUB-1                                                   L  205
      IF (IDOUB.GT.1) GO TO 295                                       L  206
      IF (L.EQ.LMAX) GO TO 295                                        L  207
      DO 190 I=1,N                                                    L  208
  190 Y(I,LMAX)=ERROR(I)                                              L  209
      GO TO 295                                                       L  210
  195 KFLAG=KFLAG-1                                                   L  211
      T=TOLD                                                          L  212
      DO 200 J1=1,NQ                                                  L  213
      DO 200 J2=J1,NQ                                                 L  214
      J=(NQ+J1)-J2                                                    L  215
      DO 200 I=1,N                                                    L  216
  200 Y(I,J)=Y(I,J)-Y(I,J+1)                                          L  217
      RMAX=2.                                                         L  218
      IF (ABS(H).LE.HMIN*1.00001) GO TO 275                           L  219
      IF (KFLAG.LE.-3) GO TO 265                                      L  220
      IREDO=2                                                         L  221
      PR3=1.E+20                                                      L  222
      GO TO 215                                                       L  223
  205 PR3=1.E+20                                                      L  224
      IF (L.EQ.LMAX) GO TO 215                                        L  225
      D1=0.                                                           L  226
      DO 210 I=1,N                                                    L  227
  210 D1=D1+((ERROR(I)-Y(I,LMAX))/YMAX(I))**2                         L  228
      ENQ3=.5/FLOAT(L+1)                                              L  229
      PR3=((D1/EUP)**ENQ3)*1.4+1.4E-6                                 L  230
  215 ENQ2=.5/FLOAT(L)                                                L  231
      PR2=((D/E)**ENQ2)*1.2+1.2E-6                                    L  232
      PR1=1.E+20                                                      L  233
      IF (NQ.EQ.1) GO TO 225                                          L  234
      D=0.                                                            L  235
      DO 220 I=1,N                                                    L  236
  220 D=D+(Y(I,L)/YMAX(I))**2                                         L  237
      ENQ1=.5/FLOAT(NQ)                                               L  238
      PR1=((D/EDN)**ENQ1)*1.3+1.3E-6                                  L  239
  225 IF (PR2.LE.PR3) GO TO 230                                       L  240
      IF (PR3.LT.PR1) GO TO 240                                       L  241
      GO TO 235                                                       L  242
  230 IF (PR2.GT.PR1) GO TO 235                                       L  243
      NEWQ=NQ                                                         L  244
      RH=1./PR2                                                       L  245
      GO TO 255                                                       L  246
  235 NEWQ=NQ-1                                                       L  247
      RH=1./PR1                                                       L  248
      GO TO 255                                                       L  249
  240 NEWQ=L                                                          L  250
```

```
      RH=1./PR3                                                          L  251
      IF (RH.LT.1.1) GO TO 250                                           L  252
      DO 245 I=1,N                                                       L  253
  245 Y(I,NEWQ+1)=ERROR(I)*EL(L)/FLOAT(L)                                L  254
      GO TO 260                                                          L  255
  250 IDOUB=10                                                           L  256
      GO TO 295                                                          L  257
  255 IF ((KFLAG.EQ.0).AND.(RH.LT.1.1)) GO TO 250                        L  258
      IF (NEWQ.EQ.NQ) GO TO 35                                           L  259
  260 NQ=NEWQ                                                            L  260
      L=NQ+1                                                             L  261
      IRET=2                                                             L  262
      GO TO 15                                                           L  263
  265 IF (KFLAG.EQ.-9) GO TO 280                                         L  264
      RH=10.**KFLAG                                                      L  265
      RH=AMAX1(HMIN/ABS(H),RH)                                           L  266
      H=H*RH                                                             L  267
      CALL DIFFUN (N,T,Y,W1)                                             L  268
      NFE=NFE+1                                                          L  269
      DO 270 I=1,N                                                       L  270
  270 Y(I,2)=H*W1(I,1)                                                   L  271
      IWEVAL=MITER                                                       L  272
      IDOUB=10                                                           L  273
      IF (NQ.EQ.1) GO TO 50                                              L  274
      NQ=1                                                               L  275
      L=2                                                                L  276
      IRET=3                                                             L  277
      GO TO 15                                                           L  278
  275 KFLAG=-1                                                           L  279
      GO TO 295                                                          L  280
  280 KFLAG=-2                                                           L  281
      GO TO 295                                                          L  282
  285 KFLAG=-3                                                           L  283
      GO TO 295                                                          L  284
  290 RMAX=100.                                                          L  285
  295 HOLD=H                                                             L  286
      JSTART=NQ                                                          L  287
      RETURN                                                             L  288
      END                                                                L  289-
```

```
      SUBROUTINE COSET (METH,NQ,EL,TQ,MAXDER)                           M    1
      DIMENSION PERTST(12,2,3), EL(13), TQ(4)                           M    2
      DATA PERTST/1.,1.,2.,1.,.3158,.07407,.01391,.002182,.0002945,.0000 M    3
     13492,.000003692,.0000003524,1.,1.,.5,.1667,.04167,1.,1.,1.,1.,1.,1 M    4
     2.,1.,2.,12.,24.,37.89,53.33,70.08,87.97,106.9,126.7,147.4,168.8,19 M    5
     31.0,2.0,4.5,7.333,10.42,13.7,1.,1.,1.,1.,1.,1.,1.,12.0,24.0,37.89, M    6
     453.33,70.08,87.97,106.9,126.7,147.4,168.8,191.0,1.,3.0,6.0,9.167,1 M    7
     52.5,1.,1.,1.,1.,1.,1.,1./                                         M    8
    5 MAXDER=5                                                          M    9
      GO TO (10,15,20,25,30),NQ                                         M   10
   10 EL(1)=1.0                                                         M   11
      GO TO 35                                                          M   12
   15 EL(1)=6.6666666666667E-01                                         M   13
      EL(3)=3.3333333333333E-01                                         M   14
      GO TO 35                                                          M   15
   20 EL(1)=5.4545454545455E-01                                         M   16
      EL(3)=EL(1)                                                       M   17
      EL(4)=9.0909090909091E-02                                         M   18
      GO TO 35                                                          M   19
   25 EL(1)=0.48                                                        M   20
      EL(3)=0.7                                                         M   21
      EL(4)=0.2                                                         M   22
      EL(5)=0.02                                                        M   23
      GO TO 35                                                          M   24
   30 EL(1)=4.3795620437956E-01                                         M   25
      EL(3)=8.2116788321168E-01                                         M   26
      EL(4)=3.1021897810219E-01                                         M   27
      EL(5)=5.4744525547445E-02                                         M   28
      EL(6)=3.6496350364964E-03                                         M   29
   35 DO 40 K=1,3                                                       M   30
   40 TQ(K)=PERTST(NQ,METH,K)                                           M   31
      TQ(4)=.5*TQ(2)/FLOAT(NQ+2)                                        M   32
      RETURN                                                            M   33
      END                                                               M   34-
```

```
      SUBROUTINE NSCORA (N,IA,JA,A,IAP,JAWORK,AWORK,C,IR,ICT)          N    1
      INTEGER IA(1),JA(1),IAP(1),JAWORK(1),C(1),IR(1),ICT(1)           N    2
      REAL A(1),AWORK(1)                                               N    3
      DO 5 K=1,N                                                       N    4
      ICK=C(K)                                                         N    5
    5 IR(ICK)=K                                                        N    6
      JMIN=1                                                           N    7
      DO 15 K=1,N                                                      N    8
      ICK=C(K)                                                         N    9
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1                                    N   10
      IF (JMIN.GT.JMAX) GO TO 15                                       N   11
      IAINK=IA(ICK)-1                                                  N   12
      DO 10 J=JMIN,JMAX                                                N   13
      IAINK=IAINK+1                                                    N   14
      JAOUTJ=JA(IAINK)                                                 N   15
      JAOUTJ=IR(JAOUTJ)                                                N   16
      JAWORK(J)=JAOUTJ                                                 N   17
   10 AWORK(J)=A(IAINK)                                                N   18
   15 JMIN=JMAX+1                                                      N   19
      DO 20 I=1,N                                                      N   20
   20 ICT(I)=IAP(I)                                                    N   21
      JMIN=1                                                           N   22
      DO 30 I=1,N                                                      N   23
      ICK=C(I)                                                         N   24
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1                                    N   25
      IF (JMIN.GT.JMAX) GO TO 30                                       N   26
      DO 25 J=JMIN,JMAX                                                N   27
      JAOUTJ=JAWORK(J)                                                 N   28
      ICTJ=ICT(JAOUTJ)                                                 N   29
      A(ICTJ)=AWORK(J)                                                 N   30
      ICT(JAOUTJ)=ICTJ+1                                               N   31
   25 CONTINUE                                                         N   32
   30 JMIN=JMAX+1                                                      N   33
      RETURN                                                           N   34
      END                                                              N   35-
```

```
      SUBROUTINE NSNFAC (N,IA,JA,A,IL,JL,ISL,L,D,IU,JU,ISU,U,X,IRL,JRL,I 0    1
     1ER)                                                                0    2
      INTEGER IA(1),JA(1),IL(1),JL(1),ISL(1)                             0    3
      INTEGER IU(1),JU(1),ISU(1),IRL(1),JRL(1)                           0    4
      REAL A(1),L(1),D(1),U(1),X(1)                                      0    5
      REAL LKI                                                           0    6
      IER=0                                                              0    7
      DO 5 K=1,N                                                         0    8
      IRL(K)=IL(K)                                                       0    9
    5 JRL(K)=0                                                           0   10
      DO 90 K=1,N                                                        0   11
      X(K)=0.                                                            0   12
      I1=0                                                               0   13
      IF (JRL(K).EQ.0) GO TO 15                                          0   14
      I=JRL(K)                                                           0   15
   10 I2=JRL(I)                                                          0   16
      JRL(I)=I1                                                          0   17
      I1=I                                                               0   18
      X(I)=0.                                                            0   19
      I=I2                                                               0   20
      IF (I.NE.0) GO TO 10                                               0   21
   15 JMIN=ISU(K)                                                        0   22
      JMAX=JMIN+IU(K+1)-IU(K)-1                                          0   23
      IF (JMIN.GT.JMAX) GO TO 25                                         0   24
      DO 20 J=JMIN,JMAX                                                  0   25
      JUJ=JU(J)                                                          0   26
   20 X(JUJ)=0.                                                          0   27
   25 JMIN=IA(K)                                                         0   28
      JMAX=IA(K+1)-1                                                     0   29
      DO 30 J=JMIN,JMAX                                                  0   30
      JAJ=JA(J)                                                          0   31
   30 X(JAJ)=A(J)                                                        0   32
      I=I1                                                               0   33
      IF (I.EQ.0) GO TO 50                                               0   34
   35 IRLI=IRL(I)                                                        0   35
      LKI=-X(I)                                                          0   36
      L(IRLI)=-LKI                                                       0   37
      JMIN=IU(I)                                                         0   38
      JMAX=IU(I+1)-1                                                     0   39
      IF (JMIN.GT.JMAX) GO TO 45                                         0   40
      ISUB=ISU(I)-1                                                      0   41
      DO 40 J=JMIN,JMAX                                                  0   42
      ISUB=ISUB+1                                                        0   43
      JUJ=JU(ISUB)                                                       0   44
   40 X(JUJ)=X(JUJ)+LKI*U(J)                                             0   45
   45 I=JRL(I)                                                           0   46
      IF (I.NE.0) GO TO 35                                               0   47
   50 IF (X(K).EQ.0.) GO TO 95                                           0   48
      DK=1./X(K)                                                         0   49
      D(K)=DK                                                            0   50
```

```
      IF (K.EQ.N) GO TO 90                                          0  51
      JMIN=IU(K)                                                    0  52
      JMAX=IU(K+1)-1                                                0  53
      IF (JMIN.GT.JMAX) GO TO 60                                    0  54
      ISUB=ISU(K)-1                                                 0  55
      DO 55 J=JMIN,JMAX                                             0  56
      ISUB=ISUB+1                                                   0  57
      JUJ=JU(ISUB)                                                  0  58
   55 U(J)=X(JUJ)*DK                                                0  59
   60 CONTINUE                                                      0  60
      I=I1                                                          0  61
      IF (I.EQ.0) GO TO 85                                          0  62
   65 IRL(I)=IRL(I)+1                                               0  63
      I1=JRL(I)                                                     0  64
      IF (IRL(I).GE.IL(I+1)) GO TO 80                               0  65
      ISLB=IRL(I)-IL(I)+ISL(I)                                      0  66
      J=JL(ISLB)                                                    0  67
   70 IF (I.GT.JRL(J)) GO TO 75                                     0  68
      J=JRL(J)                                                      0  69
      GO TO 70                                                      0  70
   75 JRL(I)=JRL(J)                                                 0  71
      JRL(J)=I                                                      0  72
   80 I=I1                                                          0  73
      IF (I.NE.0) GO TO 65                                          0  74
   85 ISLK=ISL(K)                                                   0  75
      IF (IRL(K).GE.IL(K+1)) GO TO 90                               0  76
      J=JL(ISLK)                                                    0  77
      JRL(K)=JRL(J)                                                 0  78
      JRL(J)=K                                                      0  79
   90 CONTINUE                                                      0  80
      RETURN                                                        0  81
   95 IER=K                                                         0  82
      RETURN                                                        0  83
      END                                                           0  84-
```

```
      SUBROUTINE NSBSLV (N,R,C,IL,JL,ISL,L,D,IU,JU,ISU,U,X,B,Y)          P    1
      DIMENSION R(1), IL(1), JL(1), IU(1), JU(1), C(1), ISL(1), ISU(1)  P    2
      DIMENSION L(1), X(1), B(1), U(1), Y(1), D(i)                      P    3
      INTEGER R,RK,C,CK                                                 P    4
      REAL L                                                            P    5
      DO 5 K=1,N                                                        P    6
      RK=R(K)                                                           P    7
    5 Y(K)=B(RK)                                                        P    8
      DO 15 K=1,N                                                       P    9
      JMIN=IL(K)                                                        P   10
      JMAX=IL(K+1)-1                                                    P   11
      YK=-D(K)*Y(K)                                                     P   12
      Y(K)=-YK                                                          P   13
      IF (JMIN.GT.JMAX) GO TO 15                                        P   14
      ISLB=ISL(K)-1                                                     P   15
      DO 10 J=JMIN,JMAX                                                 P   16
      ISLB=ISLB+1                                                       P   17
      JLJ=JL(ISLB)                                                      P   18
   10 Y(JLJ)=Y(JLJ)+YK*L(J)                                             P   19
   15 CONTINUE                                                          P   20
      K=N                                                               P   21
      DO 30 I=1,N                                                       P   22
      SUM=-Y(K)                                                         P   23
      JMIN=IU(K)                                                        P   24
      JMAX=IU(K+1)-1                                                    P   25
      IF (JMIN.GT.JMAX) GO TO 25                                        P   26
      ISUB=ISU(K)-1                                                     P   27
      DO 20 J=JMIN,JMAX                                                 P   28
      ISUB=ISUB+1                                                       P   29
      JUJ=JU(ISUB)                                                      P   30
   20 SUM=SUM+U(J)*Y(JUJ)                                               P   31
   25 Y(K)=-SUM                                                         P   32
      CK=C(K)                                                           P   33
      X(CK)=-SUM                                                        P   34
   30 K=K-1                                                             P   35
      RETURN                                                            P   36
      END                                                               P   37-
```

```
      SUBROUTINE YSMER (A,K,A1)                                    Q    1
      INTEGER A,A1(2)                                              Q    2
      COMMON /INOUT/ INP,LOUT,ITAPE                                Q    3
      WRITE (LOUT,5) A,K,A1(1),A1(2)                               Q    4
      RETURN                                                       Q    5
C                                                                  Q    6
C                                                                  Q    7
C                                                                  Q    8
    5 FORMAT (1X,A10,I6,2A10)                                      Q    9
      END                                                          Q   10-
```

```
      SUBROUTINE INTERP (TOUT,Y,NO,YO)                                  R    1
      COMMON /GEAR1/ T,H,DUMMY(4),N,IDUMMY(2),JSTART                    R    2
      DIMENSION YO(NO), Y(NO,1)                                         R    3
      DO 5 I=1,N                                                        R    4
    5 YO(I)=Y(I,1)                                                      R    5
      L=JSTART+1                                                        R    6
      S=(TOUT-T)/H                                                      R    7
      S1=1.                                                             R    8
      DO 15 J=2,L                                                       R    9
      S1=S1*S                                                           R   10
      DO 10 I=1,N                                                       R   11
   10 YO(I)=YO(I)+S1*Y(I,J)                                             R   12
   15 CONTINUE                                                          R   13
      RETURN                                                            R   14
      END                                                               R   15-
```

```
      SUBROUTINE SPARS (IA,JA,N)                                          S    1
      COMMON /DATA/ NR,KR(200,7),A(200),S(200),ITITLE(7),TEMP,ERR,START,  S    2
     1STOPP,PC,NP,SIG(91),IP(91),ITYPE(200),R(200),BK,SG,DILUT            S    3
      DIMENSION IA(N), JA(N)                                              S    4
      DO 5 I=1,N                                                          S    5
    5 IA(I)=1                                                             S    6
      KT=0                                                                S    7
      IA(N+1)=1                                                           S    8
      JA(1)=0                                                             S    9
      DO 70 IR=1,NR                                                       S   10
      IF (KR(IR,1).EQ.N+2) GO TO 70                                       S   11
      IF (KR(IR,1).EQ.0.OR.KR(IR,1).EQ.99) GO TO 70                       S   12
      MT=ITYPE(IR)                                                        S   13
      DO 65 K=1,MT                                                        S   14
      I=KR(IR,K)                                                          S   15
      IF (KR(IR,K).EQ.N+2) GO TO 65                                       S   16
      DO 30 L=1,MT                                                        S   17
      J=KR(IR,L)                                                          S   18
      IF (KR(IR,L).EQ.N+2) GO TO 30                                       S   19
      K1=IA(J)                                                            S   20
      K2=IA(J+1)-1                                                        S   21
      IF (K1.GT.K2) GO TO 15                                              S   22
      DO 10 M=K1,K2                                                       S   23
   10 IF (I.EQ.JA(M)) GO TO 30                                            S   24
   15 DO 20 M=J,N                                                         S   25
   20 IA(M+1)=IA(M+1)+1                                                   S   26
      KT=KT+1                                                             S   27
      KD=KT-K2                                                            S   28
      K2=K2+1                                                             S   29
      DO 25 M=1,KD                                                        S   30
   25 JA(KT+2-M)=JA(KT+1-M)                                               S   31
      JA(K2)=I                                                            S   32
   30 CONTINUE                                                            S   33
      K1=IA(I)                                                            S   34
      DO 60 L=4,7                                                         S   35
      K2=IA(I+1)-1                                                        S   36
      J=KR(IR,L)                                                          S   37
      IF (KR(IR,L).EQ.N+2) GO TO 60                                       S   38
      IF (J) 60,65,35                                                     S   39
   35 IF (K1.GT.K2) GO TO 45                                              S   40
      DO 40 M=K1,K2                                                       S   41
      IF (J.EQ.JA(M)) GO TO 60                                            S   42
   40 CONTINUE                                                            S   43
   45 DO 50 M=I,N                                                         S   44
   50 IA(M+1)=IA(M+1)+1                                                   S   45
      KT=KT+1                                                             S   46
      KD=KT-K2                                                            S   47
      K2=K2+1                                                             S   48
      DO 55 M=1,KD                                                        S   49
   55 JA(KT+2-M)=JA(KT+1-M)                                               S   50
```

```
      JA(K2)=J                                                    S   51
   60 CONTINUE                                                    S   52
   65 CONTINUE                                                    S   53
   70 CONTINUE                                                    S   54
      DO 80 I=1,N                                                 S   55
      K1=IA(I)+1                                                  S   56
      K2=IA(I+1)-1                                                S   57
      IF (K1.GT.K2) GO TO 80                                      S   58
      MT=K2-K1+1                                                  S   59
      DO 75 K=1,MT                                                S   60
      DO 75 M=K1,K2                                               S   61
      IF (JA(M).GT.JA(M-1)) GO TO 75                              S   62
      J=JA(M-1)                                                   S   63
      JA(M-1)=JA(M)                                               S   64
      JA(M)=J                                                     S   65
   75 CONTINUE                                                    S   66
   80 CONTINUE                                                    S   67
      M=N                                                         S   68
      DO 95 I=1,M                                                 S   69
      IF (IA(I+1).GT.IA(I)) GO TO 95                              S   70
      NM=I+1                                                      S   71
      NN=N+1                                                      S   72
      KMIN=IA(NM)                                                 S   73
      KMAX=IA(NN)                                                 S   74
      DO 85 J=KMIN,KMAX                                           S   75
      KM=KMAX+KMIN-J                                              S   76
   85 JA(KM)=JA(KM-1)                                             S   77
      KNOW=IA(I)                                                  S   78
      JA(KNOW)=I                                                  S   79
      DO 90 LL=NM,NN                                              S   80
   90 IA(LL)=IA(LL)+1                                             S   81
   95 CONTINUE                                                    S   82
      RETURN                                                      S   83
      END                                                         S   84-
```

```
      SUBROUTINE SORDER (N,IA,JA,P,Q,MAX,V,L,IER)                       T    1
      INTEGER IA(1),JA(1),P(1),Q(1),V(1),L(1)                           T    2
      INTEGER S,SFS,PI,PJ,PK,VI,VJ,VK,QVK,DTHR,DMIN                     T    3
      IER=0                                                             T    4
      DO 5 S=1,MAX                                                      T    5
    5 L(S)=S+1                                                          T    6
      SFS=1                                                             T    7
      L(MAX)=0                                                          T    8
      DO 10 K=1,N                                                       T    9
      P(K)=K                                                            T   10
      Q(K)=K                                                            T   11
      V(K)=1                                                            T   12
   10 L(K)=0                                                            T   13
      SFS=SFS+N                                                         T   14
      DO 50 K=1,N                                                       T   15
      JMIN=IA(K)                                                        T   16
      JMAX=IA(K+1)-1                                                    T   17
      IF (JMIN.GT.JMAX+1) GO TO 145                                     T   18
      KDIAG=0                                                           T   19
      DO 45 J=JMIN,JMAX                                                 T   20
      VJ=JA(J)                                                          T   21
      IF (VJ.NE.K) GO TO 15                                             T   22
      KDIAG=1                                                           T   23
      GO TO 45                                                          T   24
   15 LLK=K                                                             T   25
   20 LK=LLK                                                            T   26
      LLK=L(LK)                                                         T   27
      IF (LLK.EQ.0) GO TO 25                                            T   28
      IF (V(LLK)-VJ) 20,30,25                                           T   29
   25 LLK=SFS                                                           T   30
      IF (LLK.EQ.0) GO TO 150                                           T   31
      SFS=L(SFS)                                                        T   32
      V(K)=V(K)+1                                                       T   33
      V(LLK)=VJ                                                         T   34
      L(LLK)=L(LK)                                                      T   35
      L(LK)=LLK                                                         T   36
   30 LLK=VJ                                                            T   37
   35 LK=LLK                                                            T   38
      LLK=L(LK)                                                         T   39
      IF (LLK.EQ.0) GO TO 40                                            T   40
      IF (V(LLK)-K) 35,45,40                                            T   41
   40 LLK=SFS                                                           T   42
      IF (LLK.EQ.0) GO TO 150                                           T   43
      SFS=L(SFS)                                                        T   44
      V(VJ)=V(VJ)+1                                                     T   45
      V(LLK)=K                                                          T   46
      L(LLK)=L(LK)                                                      T   47
      L(LK)=LLK                                                         T   48
   45 CONTINUE                                                          T   49
      IF (KDIAG.EQ.0) GO TO 160                                         T   50
```

```
 50 CONTINUE                                                    T   51
    J=0                                                         T   52
    DTHR=0                                                      T   53
    DMIN=N                                                      T   54
    I=0                                                         T   55
 55 I=I+1                                                       T   56
    IF (I.GT.N) GO TO 140                                       T   57
    JMIN=MAXO(J+1,I)                                            T   58
    IF (JMIN.GT.N) GO TO 70                                     T   59
 60 DO 65 J=JMIN,N                                              T   60
    VI=P(J)                                                     T   61
    IF (V(VI).LE.DTHR) GO TO 75                                 T   62
    IF (V(VI).LT.DMIN) DMIN=V(VI)                               T   63
 65 CONTINUE                                                    T   64
 70 DTHR=DMIN                                                   T   65
    DMIN=N                                                      T   66
    JMIN=I                                                      T   67
    GO TO 60                                                    T   68
 75 PJ=P(I)                                                     T   69
    P(J)=PJ                                                     T   70
    Q(PJ)=J                                                     T   71
    PI=VI                                                       T   72
    P(I)=PI                                                     T   73
    Q(PI)=I                                                     T   74
    LI=VI                                                       T   75
 80 LI=L(LI)                                                    T   76
    IF (LI.EQ.0) GO TO 105                                      T   77
    VK=V(LI)                                                    T   78
    LLK=VK                                                      T   79
    LJ=VI                                                       T   80
 85 LJ=L(LJ)                                                    T   81
    IF (LJ.EQ.0) GO TO 100                                      T   82
    VJ=V(LJ)                                                    T   83
    IF (VJ.EQ.VK) GO TO 85                                      T   84
 90 LK=LLK                                                      T   85
    LLK=L(LK)                                                   T   86
    IF (LLK.EQ.0) GO TO 95                                      T   87
    IF (V(LLK)-VJ) 90,85,95                                     T   88
 95 LLK=SFS                                                     T   89
    IF (LLK.EQ.0) GO TO 155                                     T   90
    SFS=L(SFS)                                                  T   91
    V(VK)=V(VK)+1                                               T   92
    V(LLK)=VJ                                                   T   93
    L(LLK)=L(LK)                                                T   94
    L(LK)=LLK                                                   T   95
    GO TO 85                                                    T   96
100 IF (V(VK).GT.V(VI)) GO TO 80                                T   97
    I=I+1                                                       T   98
    QVK=Q(VK)                                                   T   99
    PI=P(I)                                                     T  100
```

```
      P(QVK)=PI                                                          T  101
      Q(PI)=QVK                                                          T  102
      P(I)=VK                                                            T  103
      Q(VK)=I                                                            T  104
      GO TO 80                                                           T  105
  105 LI=VI                                                              T  106
  110 IF (L(LI).EQ.0) GO TO 135                                          T  107
      LI=L(LI)                                                           T  108
      VK=V(LI)                                                           T  109
      LLK=VK                                                             T  110
      QVK=MINO(Q(VK),I)                                                  T  111
  115 LK=LLK                                                             T  112
      LLK=L(LK)                                                          T  113
      IF (LLK.EQ.0) GO TO 120                                            T  114
      VJ=V(LLK)                                                          T  115
      IF (Q(VJ).GT.QVK) GO TO 115                                        T  116
      V(VK)=V(VK)-1                                                      T  117
      L(LK)=L(LLK)                                                       T  118
      L(LLK)=SFS                                                         T  119
      SFS=LLK                                                            T  120
      LLK=LK                                                             T  121
      GO TO 115                                                          T  122
  120 IF (Q(VK).LE.I) GO TO 130                                          T  123
      IF (V(VK).LE.DTHR) GO TO 125                                       T  124
      IF ((DTHR.LT.V(VK)).AND.(V(VK).LT.DMIN)) DMIN=V(VK)                T  125
      GO TO 110                                                          T  126
  125 J=MINO(Q(VK)-1,J)                                                  T  127
      DTHR=V(VK)                                                         T  128
      GO TO 110                                                          T  129
  130 L(LK)=SFS                                                          T  130
      SFS=L(VK)                                                          T  131
      GO TO 110                                                          T  132
  135 L(LI)=SFS                                                          T  133
      SFS=L(VI)                                                          T  134
      GO TO 55                                                           T  135
  140 RETURN                                                             T  136
  145 CALL YSMER (3HROW,K,13H OF A IS NULL)                              T  137
      GO TO 165                                                          T  138
  150 CALL YSMER (3HROW,K,16H EXCEEDS STORAGE)                           T  139
      GO TO 165                                                          T  140
  155 CALL YSMER (6HVERTEX,VI,16H EXCEEDS STORAGE)                       T  141
      GO TO 165                                                          T  142
  160 CALL YSMER (6HCOLUMN,K,19H.. DIAGONAL MISSING)                     T  143
  165 IER=1                                                              T  144
      RETURN                                                             T  145
      END                                                                T  146-
```

```
      SUBROUTINE NSSFAC (N,IA,JA,MAXPL,IL,JL,ISL,MAXPU,IU,JU,ISU,P,V,IRA U     1
     1,JRA,IRAC,IRL,JRL,IRU,JRU,IER)                                    U     2
      INTEGER IA(1),JA(1),IRA(1),JRA(1),IL(1),JL(1),ISL(1)              U     3
      INTEGER IU(1),JU(1),ISU(1),IRL(1),JRL(1),IRU(1),JRU(1)            U     4
      INTEGER P(1),V(1),IRAC(1)                                         U     5
      INTEGER VI,VJ,VK,PK,PPK,PI,CEND,REND                              U     6
      IER=0                                                             U     7
      DO 5 K=1,N                                                        U     8
      IRAC(K)=0                                                         U     9
      JRA(K)=0                                                          U    10
      JRL(K)=0                                                          U    11
    5 JRU(K)=0                                                          U    12
      DO 10 K=1,N                                                       U    13
      IAK=IA(K)                                                         U    14
      IF (IAK.GT.IA(K+1)) GO TO 200                                     U    15
      IF (JA(IAK).GT.K) GO TO 10                                        U    16
      JAIAK=JA(IAK)                                                     U    17
      JRA(K)=IRAC(JAIAK)                                                U    18
      IRAC(JAIAK)=K                                                     U    19
   10 IRA(K)=IAK                                                        U    20
      JLPTR=0                                                           U    21
      IL(1)=1                                                           U    22
      JUPTR=0                                                           U    23
      IU(1)=1                                                           U    24
      DO 195 K=1,N                                                      U    25
      P(1)=1                                                            U    26
      V(1)=N+1                                                          U    27
      LSFS=2                                                            U    28
      VJ=IRAC(K)                                                        U    29
      IF (VJ.EQ.0) GO TO 30                                             U    30
   15 PPK=1                                                             U    31
   20 PK=PPK                                                            U    32
      PPK=P(PK)                                                         U    33
      IF (V(PPK)-VJ) 20,220,25                                          U    34
   25 P(PK)=LSFS                                                        U    35
      V(LSFS)=VJ                                                        U    36
      P(LSFS)=PPK                                                       U    37
      LSFS=LSFS+1                                                       U    38
      VJ=JRA(VJ)                                                        U    39
      IF (VJ.NE.0) GO TO 15                                             U    40
   30 LASTI=0                                                           U    41
      I=K                                                               U    42
   35 I=JRU(I)                                                          U    43
      IF (I.EQ.0) GO TO 60                                              U    44
      PPK=1                                                             U    45
      JMIN=IRL(I)                                                       U    46
      JMAX=ISL(I)+IL(I+1)-IL(I)-1                                       U    47
      IF (LASTI.GT.I) GO TO 40                                          U    48
      LASTI=I                                                           U    49
      LASTID=JMAX-JMIN                                                  U    50
```

```
      IF (JL(JMIN).NE.K) LASTID=LASTID+1                                U   51
   40 IF (JMIN.GT.JMAX) GO TO 35                                        U   52
      DO 55 J=JMIN,JMAX                                                 U   53
      VJ=JL(J)                                                          U   54
   45 PK=PPK                                                            U   55
      PPK=P(PK)                                                         U   56
      IF (V(PPK)-VJ) 45,55,50                                           U   57
   50 P(PK)=LSFS                                                        U   58
      V(LSFS)=VJ                                                        U   59
      P(LSFS)=PPK                                                       U   60
      PPK=LSFS                                                          U   61
      LSFS=LSFS+1                                                       U   62
   55 CONTINUE                                                          U   63
      GO TO 35                                                          U   64
   60 PI=P(1)                                                           U   65
      IF (V(PI).NE.K) GO TO 225                                         U   66
      IF (LASTI.EQ.0) GO TO 65                                          U   67
      IF (LASTID.NE.LSFS-3) GO TO 65                                    U   68
      IRLL=IRL(LASTI)                                                   U   69
      ISL(K)=IRLL+1                                                     U   70
      IF (JL(IRLL).NE.K) ISL(K)=ISL(K)-1                                U   71
      IL(K+1)=IL(K)+LASTID                                              U   72
      IRL(K)=ISL(K)                                                     U   73
      GO TO 80                                                          U   74
   65 ISL(K)=JLPTR+1                                                    U   75
      PI=P(1)                                                           U   76
      PI=P(PI)                                                          U   77
      VI=V(PI)                                                          U   78
   70 IF (VI.GT.N) GO TO 75                                             U   79
      JLPTR=JLPTR+1                                                     U   80
      IF (JLPTR.GT.MAXPL) GO TO 230                                     U   81
      JL(JLPTR)=VI                                                      U   82
      PI=P(PI)                                                          U   83
      VI=V(PI)                                                          U   84
      GO TO 70                                                          U   85
   75 IRL(K)=ISL(K)                                                     U   86
      IL(K+1)=IL(K)+JLPTR-ISL(K)+1                                      U   87
   80 P(1)=1                                                            U   88
      V(1)=N+1                                                          U   89
      LSFS=2                                                            U   90
      JMIN=IRA(K)                                                       U   91
      JMAX=IA(K+1)-1                                                    U   92
      IF (JMIN.GT.JMAX) GO TO 100                                       U   93
      DO 95 J=JMIN,JMAX                                                 U   94
      VJ=JA(J)                                                          U   95
      PPK=1                                                             U   96
   85 PK=PPK                                                            U   97
      PPK=P(PK)                                                         U   98
      IF (V(PPK)-VJ) 85,205,90                                          U   99
   90 P(PK)=LSFS                                                        U  100
```

```
      V(LSFS)=VJ                                                        U  101
      P(LSFS)=PPK                                                       U  102
   95 LSFS=LSFS+1                                                       U  103
  100 LASTI=0                                                           U  104
      I=K                                                               U  105
  105 I=JRL(I)                                                          U  106
      IF (I.EQ.0) GO TO 130                                             U  107
      PPK=1                                                             U  108
      JMIN=IRU(I)                                                       U  109
      JMAX=ISU(I)+IU(I+1)-IU(I)-1                                       U  110
      IF (LASTI.GT.I) GO TO 110                                         U  111
      LASTI=I                                                           U  112
      LASTID=JMAX-JMIN                                                  U  113
      IF (JU(JMIN).NE.K) LASTID=LASTID+1                                U  114
  110 IF (JMIN.GT.JMAX) GO TO 105                                       U  115
      DO 125 J=JMIN,JMAX                                                U  116
      VJ=JU(J)                                                          U  117
  115 PK=PPK                                                            U  118
      PPK=P(PK)                                                         U  119
      IF (V(PPK)-VJ) 115,125,120                                        U  120
  120 P(PK)=LSFS                                                        U  121
      V(LSFS)=VJ                                                        U  122
      P(LSFS)=PPK                                                       U  123
      PPK=LSFS                                                          U  124
  125 LSFS=LSFS+1                                                       U  125
      GO TO 105                                                         U  126
  130 PI=P(1)                                                           U  127
      IF (V(PI).NE.K) GO TO 210                                         U  128
      IF (LASTI.EQ.0) GO TO 135                                         U  129
      IF (LASTID.NE.LSFS-3) GO TO 135                                   U  130
      IRUL=IRU(LASTI)                                                   U  131
      ISU(K)=IRUL+1                                                     U  132
      IF (JU(IRUL).NE.K) ISU(K)=ISU(K)-1                                U  133
      IU(K+1)=IU(K)+LASTID                                              U  134
      IRU(K)=ISU(K)                                                     U  135
      GO TO 150                                                         U  136
  135 ISU(K)=JUPTR+1                                                    U  137
      PI=P(1)                                                           U  138
      PI=P(PI)                                                          U  139
      VI=V(PI)                                                          U  140
  140 IF (VI.GT.N) GO TO 145                                            U  141
      JUPTR=JUPTR+1                                                     U  142
      IF (JUPTR.GT.MAXPU) GO TO 215                                     U  143
      JU(JUPTR)=VI                                                      U  144
      PI=P(PI)                                                          U  145
      VI=V(PI)                                                          U  146
      GO TO 140                                                         U  147
  145 IRU(K)=ISU(K)                                                     U  148
      IU(K+1)=IU(K)+JUPTR-ISU(K)+1                                      U  149
  150 I=K                                                               U  150
```

```
155 I1=JRL(I)                                                          U  151
    CEND=ISL(I)+IL(I+1)-IL(I)                                          U  152
    IF (IRL(I).GE.CEND) GO TO 160                                      U  153
    IRLI=IRL(I)                                                        U  154
    J=JL(IRLI)                                                         U  155
    JRL(I)=JRL(J)                                                      U  156
    JRL(J)=I                                                           U  157
160 I=I1                                                               U  158
    IF (I.EQ.0) GO TO 165                                              U  159
    IRL(I)=IRL(I)+1                                                    U  160
    GO TO 155                                                          U  161
165 I=K                                                                U  162
170 I1=JRU(I)                                                          U  163
    REND=ISU(I)+IU(I+1)-IU(I)                                          U  164
    IF (IRU(I).GE.REND) GO TO 175                                      U  165
    IRUI=IRU(I)                                                        U  166
    J=JU(IRUI)                                                         U  167
    JRU(I)=JRU(J)                                                      U  168
    JRU(J)=I                                                           U  169
175 I=I1                                                               U  170
    IF (I.EQ.0) GO TO 180                                              U  171
    IRU(I)=IRU(I)+1                                                    U  172
    GO TO 170                                                          U  173
180 I=IRAC(K)                                                          U  174
    IF (I.EQ.0) GO TO 195                                              U  175
185 I1=JRA(I)                                                          U  176
    IRA(I)=IRA(I)+1                                                    U  177
    IF (IRA(I).GE.IA(I+1)) GO TO 190                                   U  178
    IRAI=IRA(I)                                                        U  179
    IF (JA(IRAI).GT.I) GO TO 190                                       U  180
    JAIRAI=JA(IRAI)                                                    U  181
    JRA(I)=IRAC(JAIRAI)                                                U  182
    IRAC(JAIRAI)=I                                                     U  183
190 I=I1                                                               U  184
    IF (I.NE.0) GO TO 185                                              U  185
195 CONTINUE                                                           U  186
    ISL(N)=JLPTR                                                       U  187
    ISU(N)=JUPTR                                                       U  188
    RETURN                                                             U  189
200 CALL YSMER (3HROW,K,13H OF A IS NULL)                              U  190
    GO TO 235                                                          U  191
205 CALL YSMER (3HROW,K,20H HAS DUPLICATE ENTRY)                       U  192
    GO TO 235                                                          U  193
210 CALL YSMER (3HROW,K,17H HAS A NULL PIVOT)                          U  194
    GO TO 235                                                          U  195
215 CALL YSMER (3HROW,K,19H EXCEEDS JU STORAGE)                        U  196
    GO TO 235                                                          U  197
220 CALL YSMER (3HCOL,K,20H HAS DUPLICATE ENTRY)                       U  198
    GO TO 235                                                          U  199
225 CALL YSMER (3HCOL,K,17H HAS A NULL PIVOT)                          U  200
```

```
    GO TO 235                                                    U  201
230 CALL YSMER (3HCOL,K,19H EXCEEDS JL STORAGE)                  U  202
235 IER=1                                                        U  203
    RETURN                                                       U  204
    END                                                          U  205-
```

```
      SUBROUTINE NSCORD (N,IA,JA,IAWORK,JAWORK,C,IR,ICT)                V    1
      INTEGER IA(1),JA(1),IAWORK(1),JAWORK(1),C(1),IR(1),ICT(1)         V    2
      DO 5 I=1,N                                                        V    3
    5 ICT(I)=0                                                          V    4
      IAWORK(1)=1                                                       V    5
      DO 15 K=1,N                                                       V    6
      ICK=C(K)                                                          V    7
      JMIN=IAWORK(K)                                                    V    8
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1                                     V    9
      IAWORK(K+1)=JMAX+1                                                V   10
      IF (JMIN.GT.JMAX) GO TO 15                                        V   11
      IAINK=IA(ICK)-1                                                   V   12
      DO 10 J=JMIN,JMAX                                                 V   13
      IAINK=IAINK+1                                                     V   14
      JAOUTJ=JA(IAINK)                                                  V   15
      JAOUTJ=IR(JAOUTJ)                                                 V   16
      JAWORK(J)=JAOUTJ                                                  V   17
   10 ICT(JAOUTJ)=ICT(JAOUTJ)+1                                         V   18
   15 CONTINUE                                                          V   19
      IA(1)=1                                                           V   20
      DO 20 I=1,N                                                       V   21
      IA(I+1)=IA(I)+ICT(I)                                              V   22
   20 ICT(I)=IA(I)                                                      V   23
      DO 30 I=1,N                                                       V   24
      JMIN=IAWORK(I)                                                    V   25
      JMAX=IAWORK(I+1)-1                                                V   26
      IF (JMIN.GT.JMAX) GO TO 30                                        V   27
      DO 25 J=JMIN,JMAX                                                 V   28
      JAOUTJ=JAWORK(J)                                                  V   29
      ICTJ=ICT(JAOUTJ)                                                  V   30
      JA(ICTJ)=I                                                        V   31
   25 ICT(JAOUTJ)=ICTJ+1                                                V   32
   30 CONTINUE                                                          V   33
      RETURN                                                            V   34
      END                                                               V   35-
```

```
      BLOCK DATA ALPHA1                                                 W    1
      COMMON /ALPHA/ IGO(4),IBLANK,MBLANK,JINTER                        W    2
      COMMON /APLOT/ JVERT(52,2),JBLANK,JSTAR,JPLUS,JBAR                W    3
      COMMON /GEAR1/ T,GUESS,HMIN,HMAX,EPS1,UROUND,NC,MF1,KFLAG1,JSTART W    4
      COMMON /HEAT/ CV,Q(200),SC(200,7),ISC(200,3),ITEMP                W    5
      COMMON /STORE/ AST(35),IPL(7),TEMEND,NTEMP,TMI,NPHOT,PHI,IL,NFRST, W   6
     1IPH(30),QM(100),PM(100),PSTOP                                     W    7
      COMMON /PHOTR/ IPP,RDAT(80),RTIM(80),RR1,IN10                     W    8
      DATA IGO(1)/4HMORE/,IGO(2)/4HCONT/,IGO(3)/4HPLOT/,IGO(4)/4H    /,I W    9
     1BLANK/4H    /,MBLANK/4HM   /,JINTER/4HINTV/                       W    10
      DATA JVERT/12*4H    ,4H C  ,4H O  ,4H N  ,4H C  ,4H E  ,4H N  ,4H  W    11
     1T  ,4H R  ,4H A  ,4H T  ,4H I  ,4H O  ,4H N  ,4H    ,4H P  ,4H P   W    12
     2,4H M  ,75*4H    /                                               W    13
      DATA JBLANK/4H    /,JSTAR/1H*/,JPLUS/1H+/,JBAR/1HI/               W    14
      DATA ITEMP/4HTEMP/,TEMEND/0.0/,PSTOP/0.0/,IN10/1/                 W    15
      DATA UROUND/7.5E-15/                                              W    16
      END                                                               W    17-
```

Appendix B
INPUT DATA--CHEMK FORMAT

APPENDIX B

INPUT DATA--CHEMK FORMAT

```
69          SAVE        .000324
 1  NO2                  NO    O                    1.000E+00
 2  O                    O3                         4.400E+06
 3  NO    O3             NO2                        2.39E+01    1450.0
 4  NO2   O3             NO3                        6.800E-02   2450.0
 5  NO2   O              NO                         1.340E+04
 6  OH    O3             HO2                        7.700E+01   1000.0
 7  HO2   O3             OH                         5.000E+00   1525.0
 8  OH    NO2            HNO3                       1.400E+04
 9  OH    CO             HO2   CO2                  4.400E+02
10  NO    NO             NO2   NO2                  1.500E-04
11  NO    NO3            NO2   NO2                  2.800E+04
12  NO2   NO3   H2O                                 1.560E-03   -10600.0
13  NO    HO2            NO2   OH                   1.200E+04
14  HO2   HO2                                       1.500E+04
15  O     PAR            MEO2  OH                   2.000E+01
16  OH    PAR            MEO2                       1.500E+03
17  O     OLE            MEO2  ACO3  X              2.700E+03
18  O     OLE            CARB  PAR                  2.700E+03
19  OH    OLE            RAO2                       4.200E+04
20  O3    OLE            CARB  CRIG                 8.000E-03
21  O3    OLE            CARB  MCRG  X              8.000E-03
22  O     ETH            MEO2  HO2   CO             6.000E+02
23  O     ETH            CARB  PAR                  6.000E+02
24  OH    ETH            RBO2                       1.200E+04
25  O3    ETH            CARB  CRIG                 2.400E-03
26  NO    ACO3           NO2   MEO2  CO2            3.800E+03
27  NO    RBO2           NO2   CARB  CARB  HO2      1.200E+04
28  NO    RAO2           NO2   CARB  CARB  HO2      1.200E+04
29  NO    MEO2           NO2   CARB  MEO2  X        4.000E+03
30  NO    MEO2           NO2   CARB  HO2            8.000E+03
31  NO    MEO2           NRAT                       5.000E+02
32  O3    RBO2           CARB  CARB  HO2            5.000E+00
33  O3    RAO2           CARB  CARB  HO2            2.000E+02
34  O3    MEO2           CARB  HO2                  5.000E+00
35  OH    CARB           HO2   CO                   9.500E+03
36  OH    CARB           ACO3  X                    9.500E+03
37  CARB                 QQ                         1.000E+00
38  QQ                   HO2   HO2   CO             1.000E+02
39  QQ                   MEO2  X     HO2   CO       1.000E+02
40  CARB                 CO                         3.500E-01
41  PAR   X                                         1.000E+05
42  NO2   ACO3           PAN                        2.000E+03
43  PAN                  ACO3  NO2                  2.800E-02   12500.0
44  HO2   ACO3                                      4.000E+03
45  HO2   MEO2                                      4.600E+03
46  NO    CRIG           NO2   CARB                 1.200E+04
47  NO2   CRIG           NO3   CARB                 8.000E+03
48  CARB  CRIG                                      2.000E+03
49  NO    MCRG           NO2   CARB  PAR            1.200E+04
50  NO2   MCRG           NO3   CARB  PAR            8.000E+03
51  CARB  MCRG                                      2.000E+03
52  CRIG                 CO                         5.700E+02
53  CRIG                                            2.400E+03
54  CRIG                 HO2   HO2   CO2            9.600E+01
55  MCRG                                            1.500E+02
56  MCRG                 MEO2  OH    CO             8.400E+02
57  MCRG                 MEO2  HO2   CO2            4.250E+02
58  MCRG                 CARB  HO2   HO2   CO       8.500E+01
59  OH    ARO            HO2   Y     Y     Y        6.000E+03
60  OH    ARO            HO2   GLY   X              1.600E+03
61  OH    ARO            OH    GLY   W              1.500E+04
62  CARB  W                                         1.000E+03
```

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```
 63  NO    Y          NO    CARB PAR          3.000E+01
 64  NO    Y          NO2   AERO              1.500E+01
 65  NO3   Y          CARB  CARB              3.500E+04
 66  O3    Y          AERO                    6.000E-01
 67  OH    GLY        HO2   CG    CO          1.000E+04
 68  CG              Y     Y     Y           1.000E+02
 69  GLY             MEO2  HO2   CG          2.025E-01
MORE
 70          SAVE     .000324
  1  NO2              NO    O                 .3
 37  CARB             QQ                      .00064
 40  CARB             CO                      .00032
 29  NO    MEO2       NO2   CARB  MEO2 X      2770.
 30  NO    MEO2       NO2   CARB  HO2         9230.
 69  GLY              MEO2  HO2   CG          .072
 71  RX               OH                      .03
 72                   CO                      .003
 73  O3                                       .001
 70  H2O                                      -.000324
EC-237
 10                                60.         60.
NO          NO2        OLE        PAR         AMO         CARB        H2O
RX          CO         ETH
.377        .106       .09        7.35        .177        .1012       24000.
.004        .9         .875
            360.       303.2
PLOT
EC-237
            3       0.00 0.20 0.40 0.60 0.80  0.          .8          0.          490.
O3    25 0
0.          .002       15.        .002        30.         .01         45.         .042
60.         .11        75.        .188        90.         .264        105.        .335
120.        .391       135.       .452        150.        .511        165.        .557
180.        .594       195.       .62         210.        .64         225.        .65
240.        .655       255.       .65         270.        .648        285.        .635
300.        .628       315.       .613        330.        .603        345.        .594
360.        .584
NO    25 N
0.          .377       15.        .272        30.         .169        45.         .083
60.         .04        75.        .024        90.         .018        105.        .013
120.        .011       135.       .01         150.        .007        165.        .007
180.        .006       195.       .006        210.        .006        225.        .006
240.        .006       255.       .006        270.        .005        285.        .005
300.        .005       315.       .005        330.        .005        345.        .005
360.        .005
NO2   25 2
0.          .106       15.        .198        30.         .29         45.         .353
60.         .368       75.        .35         90.         .324        105.        .297
120.        .268       135.       .234        150.        .205        165.        .171
180.        .142       195.       .117        210.        .096        225.        .07
240.        .074       255.       .068        270.        .063        285.        .05
300.        .039       315.       .038        330.        .037        345.        .037
360.        .036
                    BLANK CARD
                    BLANK CARD
```

Appendix C
INPUT DATA--EPA FORMAT

APPENDIX C

INPUT DATA--EPA FORMAT

```
 78   1   SAVE          .000324
NO2                 1     NO          O                1.000E+00
O                   2     O3                           4.400E+04
NO      O3          3     NO2                          2.390E+01   1450.
NO2     O3          4     NO3                          4.800E-02   2450.
NO2     O           5     NO                           1.340E+04
OH      O3          6     HO2                          7.700E+01   1000.
HO2     O3          7     OH                           5.000E+00   1525.
OH      NO2         8     HNO3                         1.400E+04
OH      CO          9     HO2         CO2              4.400E+02
NO      NO          10  2. NO2                          1.500E-04
NO      NO3         11  2. NO2                          2.800E+04
NO2     NO3   H2O   12                                  1.560E-03  -10600.
NO      HO2         13     NO2         OH               1.200E+04
HO2     HO2         14                                  1.500E+04
O       PAR         15     MEO2        OH               2.000E+01
OH      PAR         16     MEO2                         1.500E+03
O       OLE         17     MEO2        ACO3     X       2.700E+03
O       OLE         18     CARB        PAR              2.700E+03
OH      OLE         19     RAO2                         4.200E+04
O3      OLE         20     CARB        CRIG             8.000E-03
O3      OLE         21     CARB        MCRG     X       8.000E-03
O       ETH         22     MEO2        HO2      CO      6.000E+02
O       ETH         23     CARB        PAR              6.000E+02
OH      ETH         24     RBO2                         1.200E+04
O3      ETH         25     CARB        CRIG             2.400E-03
NO      ACO3        26     NO2         MEO2     CO2     3.800E+03
NO      RBO2        27     NO2      2. CARB     HO2     1.200E+04
NO      RAO2        28     NO2      2. CARB     HO2     1.200E+04
NO      MEO2        29     NO2         CARB     PP      4.000E+03
PP                  30     MEO2        X                1.000E+03
NO      MEO2        31     NO2         CARB     HO2     8.000E+03
NO      MEO2        32     NRAT                         5.000E+02
O3      RBO2        33  2. CARB        HO2              5.000E+00
O3      RAO2        34  2. CARB        HO2              2.000E+02
O3      MEO2        35     CARB        HO2              5.000E+00
OH      CARB        36     HO2         CO               9.500E+03
OH      CARB        37     ACO3        X                9.500E+03
CARB                38     GG          CO               1.000E+00
GG                  39  2. HO2                          1.000E+02
GG                  40     MEO2        X        HO2     1.000E+02
CARB                41     CO                           3.500E-01
PAR     X           42                                  1.000E+03
NO2     ACO3        43     PAN                          2.000E+03
PAN                 44     ACO3        NO2              2.800E-02   12500.
HO2     ACO3        45                                  4.000E+03
HO2     MEO2        46                                  4.000E+03
NO      CRIG        47     NO2         CARB             1.200E+04
NO2     CRIG        48     NO3         CARB             8.000E+03
CARB    CRIG        49                                  2.000E+03
NO      MCRG        50     NO2         CARB     PAR     1.200E+04
NO2     MCRG        51     NO3         CARB     PAR     8.000E+03
CARB    MCRG        52                                  2.000E+03
CRIG                53     CO                           6.700E+02
CRIG                54                                  2.400E+02
CRIG                55  2. HO2         CO2              9.000E+01
MCRG                56                                  1.500E+02
MCRG                57     MEO2        OH       CO      3.400E+03
MCRG                58     MEO2        HO2      CO2     4.250E+02
MCRG                59     CARB     2. HO2      CO      8.500E+01
OH      ARO         60     HO2      3. Y                6.000E+03
OH      ARO         61     HO3         GLY      X       1.400E+03
OH      ARO         62     OH          GLY      W       1.500E+04
CARB    W           63                                  1.000E+05
NO      Y           64     NO          CARB     PAR     3.000E+01
NO      Y           65     NO2         AERO             1.500E+01
NO3     Y           66  2. CARB                         3.500E+04
O3      Y           67     AERO                         6.000E-01
OH      GLY         68     HO2         CO       CO      1.000E+04
CG                  69  8. Y           MEO2     HO2     CO  2.925E-01
GLY                 70     MEO2        HO2      CO
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NORE
 74   1   SAVE          .000324
NO2                 1   NO          0                .8
CARB               38   O2          CO               .00044
CARB               41   CO                           .00032
NO      ME02       29   NO2         CARB        PF   2770.
NO      ME02       31   NO2         CARB        HO2  9230.
CLY                70   ME02        HO2         CC   .072
RX                 71   OH                           .03
                   72   CO                           .003
03                 73                                .001
H20                74                               -.000324
EC-237
  10
NO          NO2         OLE          60.        60.
RX          CO          ETH          PAR        ARO         CARB        H20
.377        .106        .09          7.35       .177        .1012       24000.
.004        .9          .675
            360.        303.2
PLOT
EC-237
     3
03   25 0          0.00 0.20 0.40 0.60 0.80  0.        .8          0.          400.
0.          .002        15.          .002        30.         .01         45.         .042
60.         .11         75.          .108        90.         .264        105.        .335
120.        .391        135.         .482        150.        .511        165.        .557
180.        .594        195.         .62         210.        .64         225.        .65
240.        .655        255.         .65         270.        .645        285.        .635
300.        .628        315.         .613        330.        .603        345.        .594
360.        .584
NO   25 N
0.          .377        15.          .272        30.         .169        45.         .083
60.         .04         75.          .024        90.         .018        105.        .013
120.        .011        135.         .01         150.        .007        165.        .007
180.        .006        195.         .006        210.        .006        225.        .006
240.        .006        255.         .006        270.        .005        285.        .005
300.        .005        315.         .005        330.        .005        345.        .005
360.        .005
NO2  25 2
0.          .106        15.          .198        30.         .29         45.         .353
60.         .368        75.          .35         90.         .324        105.        .297
120.        .268        135.         .234        150.        .205        165.        .171
180.        .142        195.         .117        210.        .096        225.        .07
240.        .074        255.         .068        270.        .063        285.        .05
300.        .039        315.         .038        330.        .037        345.        .037
360.        .036
                  BLANK CARD
                  BLANK CARD
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APPENDIX D
OUTPUT DATA

(using EPA input format for the chemical reactions)

THE REACTIONS												RATE CONSTANT	ACT. ENERGY (K)
1	NO2				→	NO	+	O				1.000E+00	-0.
2	O				→	O3						4.400E+06	-0.
3	NO	+	O3		→	NO2						2.390E+01	1.450E+03
4	NO2	+	O3		→	NO3						1.000E-02	2.450E+03
5	NO2	+	O		→	NO						1.340E+04	-0.
6	OH	+	O3		→	HO2						7.700E+01	1.000E+03
7	HO2	+	O3		→	OH						5.000E+00	1.525E+03
8	OH	+	NO2		→	HNO3						1.400E+04	-0.
9	OH	+	CO		→	HO2	+	CO2				4.400E+02	-0.
10	NO	+	NO		→	2 NO2						1.800E-04	-0.
11	NO	+	NO3		→	2 NO2						2.000E+04	-0.
12	NO2	+	NO3	+	H2O	→						1.960E-03	-1.010E+04
13	NO	+	HO2		→	NO2	+	OH				1.200E+04	-0.
14	HO2	+	HO2		→							1.800E+04	-0.
15	O	+	PAR		→	MEO2	+	CH				2.000E+01	-0.
16	OH	+	PAR		→	MEO2						1.300E+03	-0.
17	O	+	OLE		→	MEO2	+	ACOO	+	X		2.700E+03	-0.
18	O	+	OLE		→	CARB	+	PAR				2.700E+03	-0.
19	OH	+	OLE		→	RAO2						4.200E+04	-0.
20	O3	+	OLE		→	CARB	+	CRIG				0.000E-03	-0.
21	O3	+	OLE		→	CARB	+	HCHO	+	X		0.000E-03	-0.
22	O	+	ETH		→	MEO2	+	HO2	+	CO		6.000E+02	-0.
23	O	+	ETH		→	CARB	+	PAR				6.000E+02	-0.
24	OH	+	ETH		→	RBO2						1.200E+04	-0.
25	O3	+	ETH		→	CARB	+	CRIG				2.400E-03	-0.
26	NO	+	ACO3		→	NO2	+	MEO2	+	CO2		3.800E+03	-0.
27	NO	+	RBO2		→	NO2	+	2 CARB	+	HO2		1.200E+04	-0.
28	NO	+	RAO2		→	NO2	+	2 CARB	+	HO2		1.200E+04	-0.
29	NO	+	MEO2		→	NO2	+	CARB	+	PP		4.000E+03	-0.
30	PP				→	MEO2	+	X				1.000E+05	-0.
31	NO	+	MEO2		→	NO2	+	CARB	+	HO2		8.000E+03	-0.

32	NO	+	MEO2	=	MRAT					5.000E+02	-0.
33	O3	+	RNO2	=	2 CARB	+	HO2			5.000E+00	-0.
34	O3	+	RAO2	=	2 CARB	+	HO2			3.000E+02	-0.
35	O3	+	MEO2	=	CARB	+	HO2			5.000E+00	-0.
36	OH	+	CARB	=	HO2	+	CO			9.500E+03	-0.
37	OH	+	CARB	=	AC03	+	X			9.500E+03	-0.
38	CARB			=	QQ	+	CO			1.000E+00	-0.
39	QQ			=	2 HO2					1.000E+02	-0.
40	QQ			=	MEO2	+	X	+	HO2	1.000E+02	-0.
41	CARB			=	CO					3.500E-01	-0.
42	PAR	+	X	=						1.000E+05	-0.
43	NO2	+	AC03	=	PAN					2.000E+03	-0.
44	PAN			=	AC03	+	NO2			2.800E-02	1.250E+04
45	HO2	+	AC03	=						4.000E+03	-0.
46	HO2	+	MEO2	=						4.000E+03	-0.
47	NO	+	CRIC	=	NO2	+	CARB			1.200E+04	-0.
48	NO2	+	CRIC	=	NO3	+	CARB			8.000E+03	-0.
49	CARB	+	CRIC	=						2.000E+03	-0.
50	NO	+	HCRC	=	NO2	+	CARB	+	PAR	1.200E+04	-0.
51	NO2	+	HCRC	=	NO3	+	CARB	+	PAR	8.000E+03	-0.
52	CARB	+	HCRC	=						2.000E+03	-0.
53	CRIC			=	CO					6.700E+02	-0.
54	CRIC			=						2.400E+02	-0.
55	CRIC			=	2 HO2	+	CO2			9.000E+01	-0.
56	HCRC			=						1.500E+02	-0.
57	HCRC			=	MEO2	+	OH	+	CO	3.400E+02	-0.
58	HCRC			=	MEO2	+	HO2	+	CO2	4.250E+02	-0.
59	HCRC			=	CARB	+	2 HO2	+	CO	8.500E+01	-0.
60	OH	+	ARO	=	HO2	+	3 Y			6.000E+03	-0.
61	OH	+	ARO	=	HO2	+	GLY	+	X	1.600E+03	-0.
62	OH	+	ARO	=	OH	+	GLY	+	W	1.500E+04	-0.
63	CARB	+	W	=						1.000E+05	-0.

64	NO	+	Y	=	NO	+	CARB	+	PAR		5.000E+01	-0.
65	NO	+	Y	=	NO2	+	AERO				1.500E+01	-0.
66	NO3	+	Y	=	2 CARB						3.500E+04	-0.
67	O3	+	Y	=	AERO						6.000E-01	-0.
68	OH	+	CLY	=	HO2	+	CC	+	CO		1.000E+04	-0.
69	CC			=	3 Y						1.000E+02	-0.
70	CLY			=	MEO2	+	HO2	+	CC		2.025E-01	-0.

THE REACTIONS									RATE CONSTANT	ACT. ENERGY (K)
1	NO2			•	NO	+	O		3.000E-01	-0.
38	CARB			•	QQ	+	CO		6.400E-04	-0.
41	CARB			•	CO				3.200E-04	-0.
29	NO	+	MEO2	•	NO2	+	CARB	+ PP	2.770E+03	-0.
31	NO	+	MEO2	•	NO2	+	CARB	+ HO2	9.230E+03	-0.
70	GLY			•	MEO2	+	HO2	+ CC	7.260E-02	-0.
71	RX			•	OH				3.000E-02	-0.
72				•	CO				3.000E-03	-0.
73	O3			•					1.000E-03	-0.
74	H2O			•					-3.240E-04	-0.

EC-237

INITIAL CONCENTRATION

NO	NO2	OLE	PAR	ARO	CARB	H2O	RX	CO	ETH
3.770E-01	1.060E-01	9.000E-02	7.350E+00	1.770E-01	1.012E-01	2.400E+04	4.000E-03	9.000E-01	8.750E-01

THE TEMPERATURE OF THE CELL WAS = 3.03E+02 AND THE ERROR TOLERANCE = 1.00E-02

THE OVERALL DILUTION RATE WAS 5.24E-04

THE RATE CONSTANTS USED WERE

3.000E-01	4.400E+06	2.598E+01	5.527E-02	1.340E+04	8.156E+01	5.459E+00	1.400E+04	4.400E+02	1.500E-04
2.000E+04	8.476E-04	1.200E+04	1.500E+04	2.000E+01	1.500E+03	2.700E+03	2.700E+03	4.200E+04	8.000E-00
8.000E-03	6.000E+02	6.000E+03	1.200E+04	2.400E-03	3.800E+03	1.200E+04	1.200E+04	2.770E+03	1.000E+00
9.230E+03	5.000E+02	5.000E+00	2.000E+02	5.000E+00	9.500E+03	9.500E+03	6.400E-04	1.000E+02	1.000E+03
3.200E-04	1.000E+05	2.000E+03	5.749E-02	4.000E+03	4.000E+03	1.200E+04	8.000E+03	2.000E+05	1.200E+04
8.000E+03	2.000E+03	6.700E+02	2.400E+03	9.000E+01	1.500E+02	3.400E+02	4.250E+02	8.500E+01	6.000E+00
1.600E+03	1.500E+04	1.000E+05	3.000E+01	1.500E+01	3.500E+04	6.000E-01	1.000E+04	1.000E+02	1.000E-02
3.000E-02	3.000E-03	1.000E-03	-3.240E-04						

TI... IN...	NO2 H2O ETH AERO	NO PAR RNO2 CC	O MEO2 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH X PAN	HO2 CARB ARO	HNO3 RAO2 Y	CO CRIC CLY	CHC MCIC W
0.	1.060E-01	3.770E-01	0.	0.	0.	0.	0.	0.	9.000E-01	0.
1.0... -10	2.400E+04	7.350E+00	0.	9.000E-02	0.	0.	1.012E-01	0.	0.	0.
	8.750E-01	0.	0.	0.	0.	0.	1.770E-01	0.	0.	0.
	0.	0.	4.000E-03	3.032E+02	2.401E+04					
NET RA...	-3.179E-02	3.164E-02	3.180E-02	0.	0.	1.200E-04	0.	0.	2.000E-03	0.
	0.	-2.381E-03	0.	-2.916E-05	0.	0.	-1.299E-04	0.	0.	0.
	-2.835E-04	0.	0.	0.	6.477E-05	0.	-5.735E-03	0.	0.	0.
	0.	0.	-1.213E-04	0.	3.163E-02					

THE R... TION RATES ARE

3.1...-02	0.	0.	0.	0.	0.	0.	0.	0.	
0.	0.	0.	0.	0.	0.	0.	0.	0.	2.13E-05
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
3.2...-03	0.	0.	0.	0.	0.	0.	6.48E-05	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
1.2...-04	3.00E-03	0.	0.	0.	0.	0.	0.	0.	0.
			-7.78E+00						0.

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TIME INTERVAL	NO2	NO	O	O3	NO3	OH	HO2	HNO3	CO	CO2
	H2O	PAR	HE02	OLE	AC03	X	CARB	RA02	CRIC	HCRC
	ETH	HO02	PP	NRAT	QQ	PAN	ARO	Y	GLY	W
	AERO	CC	RX	TEMP	M					
6.000E+01	3.902E-01	5.125E-02	2.656E-08	8.206E-02	1.263E-06	9.331E-08	5.434E-06	2.207E-02	1.006E+00	1.422E-02
6.426E+00	2.400E+04	7.121E+00	2.710E-06	6.601E-02	3.900E-07	1.231E-09	3.430E-01	4.053E-07	3.600E-08	8.981E-09
	7.927E-01	1.421E-06	3.910E-07	4.363E-03	1.097E-06	4.001E-03	1.509E-01	2.603E-04	1.166E-02	6.152E-09
	1.097E-02	1.360E-06	6.450E-04	3.032E+02	2.401E+04					
RT RATES	-5.523E-04	-4.603E-04	-1.076E-08	3.437E-03	7.507E-05	-5.342E-05	1.030E-03	5.023E-04	3.200E-03	1.612E-04
	-1.002E-05	-3.724E-03	2.876E-03	-3.762E-04	8.930E-07	-4.006E-08	3.300E-03	2.745E-06	-6.031E-08	-6.731E-08
	-1.326E-03	1.284E-03	-5.936E-06	6.023E-05	1.143E-08	1.897E-04	-3.672E-04	1.990E-05	9.319E-05	2.433E-07
	2.159E-04	1.120E-08	-1.950E-03	0.	6.740E-03					

THE REACTION RATES ARE

1.17E-01	1.17E-01	1.03E-01	1.77E-03	1.39E-04	6.25E-07	2.43E-06	3.10E-04	4.46E-03	3.94E-07
1.81E-03	1.00E-05	3.34E-03	4.43E-07	3.78E-06	9.97E-04	4.73E-06	4.73E-06	2.59E-04	4.37E-05
4.33E-05	1.26E-05	1.26E-03	8.08E-04	1.36E-04	1.17E-04	8.74E-04	2.49E-04	3.86E-04	3.92E-06
1.29E-03	6.96E-05	5.83E-07	6.63E-06	1.12E-06	3.04E-04	3.04E-04	2.20E-04	1.10E-04	1.10E-04
1.10E-04	8.76E-04	4.67E-04	2.76E-04	1.30E-08	5.91E-08	2.24E-03	1.15E-04	2.52E-05	4.92E-06
2.50E-05	5.49E-06	2.47E-05	8.03E-06	3.31E-06	1.20E-06	2.72E-06	3.40E-06	6.80E-07	8.45E-06
2.23E-03	2.11E-04	2.11E-04	4.13E-04	2.06E-04	1.19E-05	1.32E-03	1.09E-03	1.37E-04	1.54E-04
1.94E-03	3.00E-03	8.21E-03	-7.70E+00						

TIME INTERVAL	NO2	NO	O	O3	NO3	OH	HO2	HNO3	CO	CO2
	H2O	PAR	HE02	OLE	AC03	X	CARB	RA02	CRIC	HCRC
	ETH	HO02	PP	NRAT	QQ	PAN	ARO	Y	GLY	W
	AERO	CC	RX	TEMP	M					
1.200E+02	3.429E-01	8.941E-03	2.335E-08	8.014E-01	2.793E-05	1.112E-07	5.039E-05	5.446E-02	1.299E+00	2.100E-02
4.339E+00	2.400E+04	6.875E+00	1.831E-03	3.927E-02	2.900E-06	2.043E-09	5.834E-01	1.017E-06	1.317E-07	2.403E-08
	6.981E-01	8.309E-06	4.546E-07	8.792E-03	1.067E-06	2.558E-02	1.290E-01	5.107E-04	1.563E-02	3.685E-09
	2.396E-02	1.862E-06	1.057E-04	3.032E+02	2.401E+04					
RT RATES	-2.138E-03	1.239E-06	-1.712E-08	5.106E-03	1.984E-05	-1.029E-05	3.036E-06	5.160E-04	3.831E-03	1.792E-04
	-1.930E-04	-4.563E-03	5.170E-06	-4.485E-04	1.421E-06	5.681E-09	4.364E-03	-3.011E-08	-1.260E-07	-8.570E-08
	-1.816E-03	3.182E-06	-1.125E-06	7.900E-05	1.400E-08	5.100E-04	-3.660E-04	-5.277E-06	4.607E-05	3.446E-08
	1.776E-04	6.849E-09	-5.206E-06	0.	5.358E-03					

THE REACTION RATES ARE

1.45E-01	1.03E-01	8.86E-02	7.23E-03	1.07E-04	3.46E-06	7.99E-03	5.34E-04	6.35E-05	1.24E-08
7.00E-03	1.95E-04	4.12E-03	2.21E-05	3.21E-06	1.15E-03	2.52E-06	2.52E-06	1.07E-04	1.32E-04
1.22E-04	9.70E-06	9.70E-06	9.31E-04	6.39E-04	9.05E-05	9.13E-04	1.09E-04	4.53E-04	4.53E-04
1.31E-03	8.19E-03	1.62E-05	7.76E-03	3.49E-03	6.16E-04	6.16E-04	3.73E-04	1.07E-04	1.47E-04
1.07E-04	1.40E-03	1.99E-03	1.47E-03	4.43E-07	2.81E-06	1.63E-03	4.16E-04	1.77E-04	2.04E-04
6.67E-03	2.81E-05	1.02E-04	3.64E-03	1.37E-03	3.65E-06	8.27E-06	1.03E-05	2.07E-06	8.44E-06
2.30E-03	2.13E-04	2.13E-04	1.37E-04	6.83E-03	5.00E-04	1.17E-04	1.74E-03	1.06E-04	1.69E-04
3.17E-06	3.00E-03	3.81E-04	-7.70E+00						

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TIME INTERVAL	NO2 H2O ETH AERO	NO PAR RBO2 CC	O MEO2 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH X PAR	HO2 CARB ARO	HNO3 RAO2 Y	CO CRIC GLY	CO2 MCRG W
1.[illegible]-02	2.005E-01	2.864E-03	1.366E-01	6.353E-01	7.993E-05	1.083E-07	1.070E-04	7.935E-02	1.843E+00	3.294E-02
8.[illegible]-03	2.400E+04	6.588E+00	5.258E-05	1.777E-02	1.095E-05	2.487E-09	8.214E-01	5.015E-07	2.294E-07	2.113E-08
	5.847E-01	2.022E-03	4.185E-09	1.317E-02	2.629E-06	6.997E-02	1.085E-01	2.463E-04	1.600E-02	2.140E-09
	3.180E-03	2.006E-06	1.698E-03	3.032E+02	2.401E+04					
NET RATES	-2.572E-03	5.724E-03	-6.326E-08	3.099E-03	1.468E-05	-1.130E-05	5.627E-06	2.709E-04	4.247E-03	2.110E-04
	-3.263E-04	-4.705E-03	6.356E-06	-2.607E-04	1.144E-05	-1.753E-07	3.209E-03	8.051E-09	-1.166E-07	-1.072E-07
	-1.832E-03	1.978E-06	-1.423E-06	7.093E-05	1.031E-08	6.914E-04	-3.012E-04	-1.627E-06	-1.066E-03	1.032E-07
	9.420E-05	-2.195E-09	-5.149E-07	0.	1.869E-03					

THE REACTION RATES ARE

6.[illegible]-02	6.01E-02	4.73E-02	7.05E-03	3.67E-03	5.62E-06	3.74E-04	3.05E-04	7.37E-05	1.23E-09
6.[illegible]-03	3.26E-04	3.71E-03	1.74E-04	1.80E-06	1.07E-03	6.56E-07	6.56E-07	8.10E-03	9.03E-05
9.[illegible]-03	4.79E-06	4.79E-06	7.61E-04	8.92E-04	1.19E-04	6.95E-04	1.72E-05	4.17E-04	4.19E-06
1.[illegible]-03	7.53E-05	6.43E-03	6.37E-03	1.67E-04	8.47E-04	8.47E-04	5.26E-04	2.63E-04	2.63E-06
2.[illegible]-04	1.64E-03	4.30E-03	3.68E-03	4.72E-06	2.27E-05	7.09E-06	3.68E-04	3.77E-04	7.26E-07
3.[illegible]-03	3.47E-05	1.54E-04	3.51E-05	2.06E-03	3.17E-06	7.10E-06	8.90E-06	1.80E-06	7.06E-05
1.[illegible]-03	1.77E-04	1.76E-04	2.12E-05	1.06E-03	6.90E-04	9.39E-05	1.83E-05	2.01E-04	1.82E-04
5.09E-07	3.00E-03	6.35E-04	-7.78E+00						

TIME INTERVAL	NO2 H2O ETH AERO	NO PAR RBO2 CC	O MEO2 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH X PAR	HO2 CARB ARO	HNO3 RAO2 Y	CO CRIC GLY	CO2 MCRG W
2.[illegible]-02	7.959E-02	9.527E-04	5.435E-09	7.188E-01	9.811E-05	7.010E-08	1.667E-04	8.029E-02	1.796E+00	4.369E-02
8.[illegible]-03	2.400E+04	6.323E+00	9.441E-05	7.103E-03	3.873E-03	1.960E-09	9.567E-01	1.946E-07	2.460E-07	1.147E-08
	4.060E-01	2.710E-03	2.496E-09	1.683E-03	3.061E-06	9.900E-02	9.412E-02	1.500E-04	1.440E-02	1.034E-09
	3.629E-02	1.666E-06	3.759E-06	3.032E+02	2.401E+04					
NET RATES	-1.421E-03	-1.986E-05	-3.900E-08	-1.379E-04	-2.499E-06	-1.769E-06	2.043E-07	4.931E-03	4.100E-03	2.088E-04
	-1.593E-04	-3.945E-03	3.003E-06	-1.051E-04	3.975E-05	-1.835E-07	1.365E-03	2.527E-08	-2.466E-08	-1.208E-08
	-1.408E-03	3.043E-07	-4.673E-07	3.932E-05	4.372E-09	3.990E-04	-1.796E-04	-7.339E-07	-6.176E-03	4.778E-08
	5.867E-05	-1.273E-09	-8.368E-08	0.	-1.182E-03					

THE REACTION RATES ARE

2.[illegible]-02	2.39E-02	1.78E-02	3.16E-03	5.79E-06	4.11E-06	6.54E-04	7.81E-05	5.54E-05	1.36E-10
2.[illegible]-03	1.59E-04	1.91E-03	4.17E-04	6.88E-07	6.62E-04	1.04E-07	1.04E-07	2.09E-03	4.09E-05
4.[illegible]-03	1.58E-06	1.58E-06	4.09E-04	8.38E-04	1.40E-04	3.11E-04	1.54E-06	2.49E-04	2.50E-04
8.[illegible]-04	4.50E-05	9.77E-05	1.94E-03	3.39E-04	6.37E-04	6.37E-04	6.12E-04	3.06E-04	3.06E-04
3.[illegible]-04	1.24E-03	6.17E-03	5.74E-03	2.30E-05	6.30E-05	2.82E-06	1.57E-04	4.72E-04	1.31E-07
7.31E-06	2.20E-05	1.65E-04	5.92E-05	2.22E-03	1.72E-06	2.90E-06	4.80E-06	9.75E-07	3.96E-05
1.[illegible]-05	9.90E-05	9.89E-03	4.82E-06	2.26E-06	5.44E-04	6.81E-05	1.02E-05	1.67E-04	1.56E-04
8.23E-08	3.00E-03	7.19E-04	-7.78E+00						

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TIME INTERVAL	NO2 H2O ETH AERO	NO PAR RNO2 CO	O HCO2 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH X PAN	HO2 CARB ARO	HNO3 RAD2 Y	CO CRIG CLY	CO2 [illegible] k
3.000E+02	2.264E-02	2.090E-04	1.343E-03	6.529E-01	6.033E-03	3.605E-08	1.046E-04	8.871E-02	2.032E+00	5.704E-02
4.336E+00	2.400E+04	6.113E+00	1.371E-04	3.142E-03	1.459E-04	1.313E-09	1.001E+00	3.623E-08	2.093E-07	5.149E-09
	4.153E-01	2.724E-03	1.102E-03	1.037E-02	3.264E-06	1.141E-01	8.602E-02	1.610E-04	1.043E-02	4.741E-10
	3.937E-02	1.165E-06	4.868E-07	3.032E+02	2.401E+04					
NET RATES	-4.673E-04	-8.774E-06	-2.665E-03	-1.754E-03	-1.303E-06	-2.179E-08	-4.169E-07	-1.706E-03	3.767E-03	1.959E-04
	-2.778E-03	-3.119E-03	5.059E-07	-3.073E-03	3.907E-05	-3.208E-08	2.431E-04	3.638E-09	1.764E-08	2.931E-09
	-9.698E-04	-2.048E-08	-9.272E-08	1.392E-03	7.816E-10	6.102E-06	-9.931E-05	1.312E-06	-6.721E-05	7.736E-09
	5.100E-05	-4.024E-09	-1.305E-08	0.	-2.233E-03					

THE REACTION RATES ARE

6.79E-03	6.79E-03	4.92E-03	8.17E-04	4.60E-07	1.96E-06	6.30E-04	1.17E-05	3.29E-03	1.26E-11
4.90E-04	3.70E-05	6.42E-04	5.11E-04	1.09E-07	3.30E-04	1.31E-08	1.31E-08	4.06E-06	1.64E-03
1.64E-05	5.05E-07	3.03E-07	1.04E-04	6.51E-04	1.61E-04	9.47E-05	1.26E-07	1.10E-04	1.10E-04
3.67E-04	1.99E-03	8.09E-03	4.73E-06	4.40E-04	3.51E-04	3.51E-04	6.41E-04	3.20E-04	3.20E-04
3.20E-04	8.03E-04	6.60E-03	6.56E-03	1.00E-04	1.01E-04	7.28E-07	3.79E-05	4.19E-04	1.79E-08
9.32E-07	1.03E-03	1.40E-04	5.02E-05	1.80E-03	7.72E-07	1.73E-06	2.19E-06	4.38E-07	1.90E-03
5.87E-06	4.70E-03	4.73E-03	1.40E-06	7.00E-07	3.40E-04	6.31E-03	3.04E-06	1.16E-04	1.13E-04
1.37E-08	3.00E-03	6.53E-04	-7.70E+00						

TIME INTERVAL	NO2 H2O ETH AERO	NO PAR RNO2 CO	O HCO2 PP RX	O3 OLE NRAT TEMP	NO3 ACO3 QQ M	OH X PAN	HO2 CARB ARO	HNO3 RAD2 Y	CO CRIG CLY	CO2 [illegible] k
3.670E+03	9.249E-03	1.356E-04	6.303E-10	5.423E-01	2.466E-03	2.366E-08	1.760E-04	8.733E-02	2.250E+00	6.924E-02
3.817E+00	3.400E+04	5.943E+00	1.634E-04	1.610E-03	3.244E-04	1.035E-09	9.978E-01	1.460E-08	1.573E-07	2.283E-09
	3.662E-01	2.396E-03	6.141E-10	1.801E-02	3.193E-06	1.074E-01	8.116E-02	2.212E-04	6.933E-03	2.806E-10
	4.200E-02	7.632E-07	7.491E-08	3.032E+02	2.401E+04					
NET RATES	-4.303E-03	-4.622E-07	-3.493E-11	-1.726E-03	-1.941E-07	2.199E-09	-1.033E-07	-2.523E-03	3.338E-03	1.823E-04
	-4.640E-06	-2.749E-03	1.162E-07	-1.610E-03	1.373E-06	-3.819E-10	-2.710E-04	-1.060E-10	5.201E-09	4.375E-10
	-6.994E-04	-4.624E-08	-4.022E-09	4.979E-06	-8.664E-10	-2.077E-04	-6.960E-05	-2.000E-07	-4.609E-05	1.827E-10
	5.836E-05	-5.095E-09	-2.272E-09	0.	-2.075E-03					

THE REACTION RATES ARE

2.77E-03	2.77E-03	1.91E-03	2.77E-04	7.01E-08	1.05E-06	5.21E-04	3.06E-06	2.34E-03	2.76E-12
9.37E-03	4.64E-06	2.07E-04	4.63E-04	7.49E-08	2.11E-04	2.73E-09	2.73E-09	1.61E-06	7.02E-06
7.02E-06	1.39E-07	1.39E-07	1.04E-04	4.77E-04	1.67E-04	5.90E-05	2.58E-08	6.14E-05	6.14E-05
2.03E-04	1.11E-05	6.30E-05	1.30E-06	4.43E-04	2.24E-04	2.24E-04	6.39E-04	3.19E-04	3.19E-04
3.19E-04	6.15E-04	6.00E-03	6.17E-03	2.20E-04	1.15E-04	2.56E-07	1.17E-05	3.14E-04	3.72E-09
1.69E-07	4.56E-06	1.05E-04	3.78E-05	1.42E-03	3.49E-07	7.77E-07	9.71E-07	1.94E-07	1.15E-05
3.07E-06	2.00E-03	2.00E-03	9.00E-07	4.30E-07	1.91E-04	7.20E-03	1.64E-06	7.65E-03	7.47E-05
2.25E-09	3.00E-03	5.42E-04	-7.70E+00						

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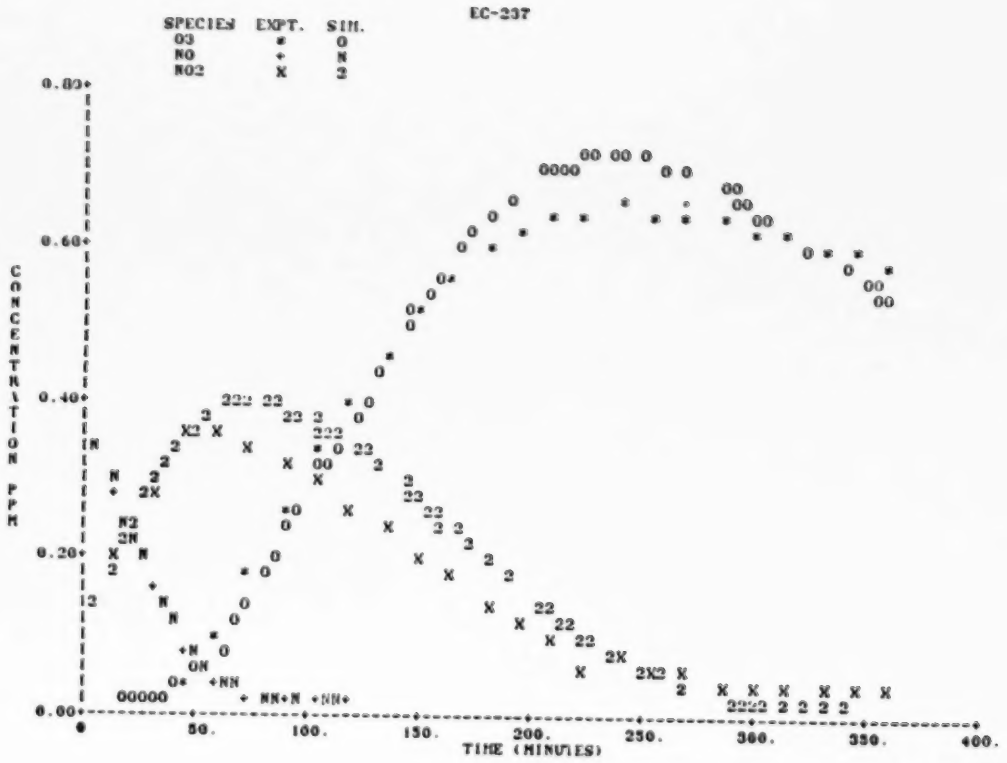

EC-237
SPECIES EXPT. SIM.
O3 * O
NO + N
NO2 X 2
CONCENTRATION PPM
0.80
0.60
0.40
0.20
0.00
0.
50.
100.
150.
200.
250.
300.
350.
400.
TIME (MINUTES)

Appendix E

EXAMPLE USE OF VARIABLE PHOTOLYSIS AND PRINT OPTIONS

APPENDIX E

EXAMPLE USE OF VARIABLE PHOTOLYSIS AND PRINT OPTIONS

```
32  1                                    14  60   7                1
      1          12          17          18          19          24          25
.016      .13       .29       .39       .46       .5        .82
.33       .82       .5        .46       .39       .29       .13
 016
NO2                   1       NO          0                   1.
O                     2       O3.                             4400000.
 3       NO           3       NO2                             23.8        1450.
NO2      O3           4       NO3                             .0474       2450.
NO2      O            5       NO                              13000.
 O3      NO           62.     NO2                             28000.
NO2      NO3          7       N2O5                            3910.       -861.
 2O5                   8       NO2         NO3                 6.85        10320.
 2O5                   92.     HNO3                            .02
NO       NO2          102.    HONO                            .0000003
HONO     HONO         11      NO          NO2                 .000015
HONO                  12      OH          NO                  .18
OH       NO2          13      HNO3                            16000.
OH       NO           14      HONO                            16000.
HO2      NO           15      NO2         OH                  12000.
HO2      HO2          16      HOOH                            7400.
HOOH                  172.    OH                              .00079
O3                    18      O1D                             .0027
O3                    19      O                               .069
O1D                   20      O                                  4.45E10 -97.4
O1D                   212.    OH                                  6.8E09
OH       O3           22      HO2                             76.9        1000.
O3       HO2          23      OH                              2.93        580.
HCHO                  24                                      .0046
HCHO                  252.    HO2                             .003
HCHO     OH           26      HO2                             14000.
MEO2     NO           28      MEO         NO2                 12000.
MEO                   29      HCHO        HO2                 200000.
MEO      NO2          30                                      15000.
MEO      NO2          31      HCHO        HONO                4400.
MEO2     HO2          32                                      7400.
REACTIVITY 1000 PPMC METHANE
  3                                 60.         60.
NO          NO2         CH4
.1          .1          1000.
            840.        303.        .01
PLOT
REACTIVITY 1000 PPMC METHANE
      1          0.00 0.40 0.80 1.20 1.40 0.         1.6         0.          880.
O3        0
          BLANK CARD
          BLANK CARD
```

									RATE CONSTANT	ACT. ENERGY (K)
1	NO2			•		NO	+	O	1.000E+00	-0.
2	O			•		O3			4.400E+06	-0.
3	O3	+	NO	•		NO2			2.300E+01	1.450E+03
4	NO2	+	O3	•		NO3			4.740E-02	2.450E+03
5	NO2	+	O	•		NO			1.300E+04	-0.
6	NO3	+	NO	•	2	NO2			2.800E+04	-0.
7	NO2	+	NO3	•		N2O5			3.910E+03	-8.610E+02
8	N2O5			•		NO2	+	NO3	6.850E+00	1.032E+04
9	N2O5			•	2	HNO3			2.000E-02	-0.
10	NO	+	NO2	•	2	HONO			3.000E-07	-0.
11	HONO	+	HONO	•		NO	+	NO2	1.500E-05	-0.
12	HONO			•		OH	+	NO	1.800E-01	-0.
13	OH	+	NO2	•		HNO3			1.600E+04	-0.
14	OH	+	NO	•		HONO			1.600E+04	-0.
15	HO2	+	NO	•		NO2	+	OH	1.200E+04	-0.
16	HO2	+	HO2	•		HOOH			7.400E+03	-0.
17	HOOH			•	2	OH			7.900E-04	-0.
18	O3			•		O1D			2.700E-03	-0.
19	O3			•		O			6.900E-02	-0.
20	O1D			•		O			4.450E+10	-9.740E+01
21	O1D			•	2	OH			6.800E+09	-0.
22	OH	+	O3	•		HO2			7.690E+01	1.000E+03
23	O3	+	HO2	•		OH			2.930E+00	5.800E+02
24	HCHO			•					4.600E-04	-0.
25	HCHO			•	2	HO2			3.000E-03	-0.
26	HCHO	+	OH	•		HO2			1.400E+04	-0.
27	CH4	+	OH	•		MEO2			1.110E+01	1.710E+03
28	MEO2	+	NO	•		MEO	+	NO2	1.200E+04	-0.
29	MEO			•		HCHO	+	HO2	2.000E+03	-0.
30	MEO	+	NO2	•					1.500E+04	-0.
31	MEO	+	NO2	•		HCHO	+	HONO	4.400E+03	-0.
32	MEO2	+	HO2	•					7.400E+03	-0.

REACTIVITY 1000 PPMC METHANE

INITIAL CONCENTRATION

NO	NO2	CH4
1.000E-01	1.000E-01	1.000E+03

THE TEMPERATURE OF THE CELL WAS = 3.03E+02 AND THE ERROR TOLERANCE = 1.00E-02

THE RATE CONSTANTS USED WERE

1.000E+00	4.400E+06	2.579E+01	5.429E-01	1.300E+04	2.000E+04	3.728E+03	1.213E+01	2.000E-02	3.000E-07
1.500E-03	1.000E-01	1.600E+04	1.600E+04	1.200E+04	7.400E+03	7.900E-04	2.700E-03	6.900E-02	4.426E+10
6.000E+09	8.120E+01	3.026E+00	4.600E-03	3.000E-03	1.400E+04	1.220E+01	1.200E+04	2.000E+05	1.500E+04
4.400E+03	7.400E+03								

THE PHOTOLYSIS REACTIONS ARE

1	12	17	18	19	24	25

THE PHOTOLYSIS RATIOS OF EACH OF THE REACTIONS ABOVE ARE

1.000E+00	1.000E-01	7.900E-04	2.700E-03	6.900E-02	4.600E-03	3.000E-03

THE NO2 PHOTOLYSIS NUMBERS IN INTERVALS OF 60 TIME UNITS ARE

1.600E-02	1.300E-01	2.900E-01	3.900E-01	4.600E-01	5.000E-01	5.200E-01	5.300E-01	5.200E-01	5.000E-01
4.600E-01	3.900E-01	2.900E-01	1.300E-01	1.600E-02					

Output Results (Continued)

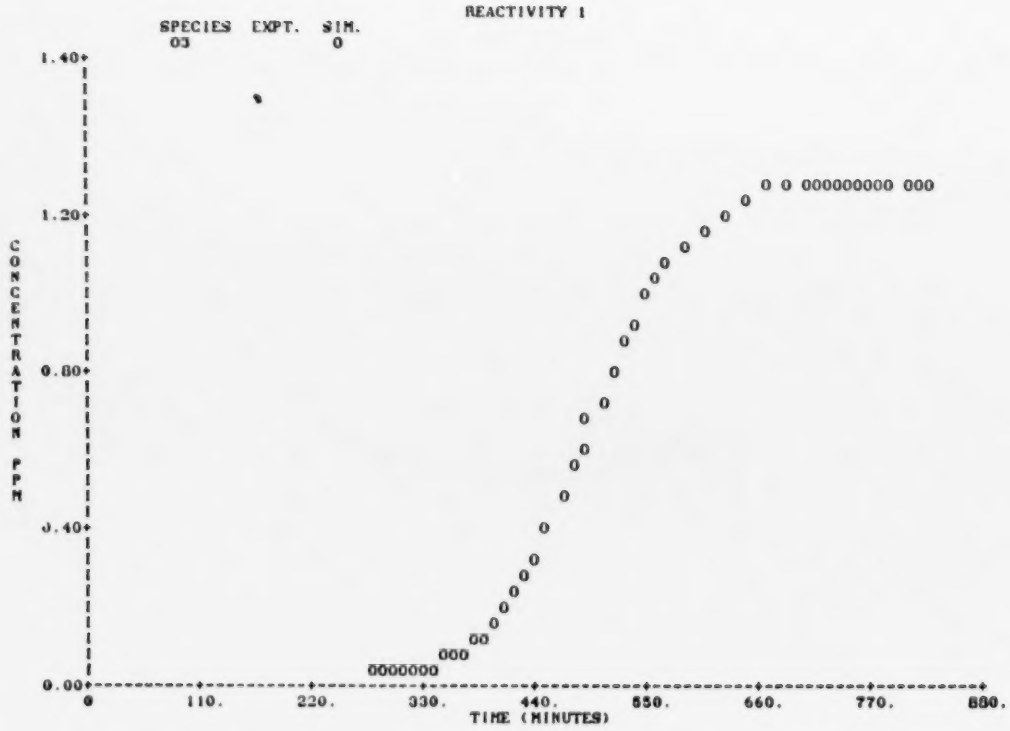
T INI	NO2 HOOH	NO O1D	O HCHO	O3 CH4	NO3 MEO2	N2O5 MEO	HNO3 TEMP	HONO M	OH	HO2
0. 1.0	1.000E-01 0.	1.000E-01 0.	0. 0.	0. 1.000E+03	0. 0.	0. 0.	0. 3.030E+02	0. 1.000E+03	0.	0.
6. 3.	9.329E-02 2.244E-13	1.047E-01 5.127E-17	2.825E-09 3.924E-03	4.551E-03 1.000E+03	8.020E-09 1.641E-09	2.344E-07 1.022E-11	5.382E-06 3.030E+02	4.444E-06 1.000E+03	1.690E-10	1.651E-09
1. 3.	9.070E-02 2.012E-11	1.092E-01 1.427E-16	6.023E-09 4.579E-04	9.301E-03 1.000E+03	1.497E-08 1.221E-08	4.165E-07 7.930E-11	5.960E-03 3.030E+02	3.064E-03 1.000E+03	1.311E-09	1.272E-08
1. 1.	9.025E-02 3.794E-10	1.093E-01 2.561E-16	8.073E-09 2.200E-03	1.213E-02 1.000E+03	1.988E-08 4.205E-08	5.502E-07 2.790E-10	2.898E-04 3.030E+02	9.503E-05 1.000E+03	4.614E-09	4.647E-08
2. 1.	9.688E-02 4.490E-09	1.017E-01 4.108E-16	1.023E-08 7.586E-03	1.689E-02 1.000E+03	3.113E-08 1.409E-07	9.237E-07 8.533E-10	1.069E-03 3.030E+02	2.414E-04 1.000E+03	1.412E-08	1.579E-07
4. 4.	1.176E-01 5.230E-08	7.810E-02 7.631E-16	1.359E-08 2.164E-02	2.086E-02 1.000E+03	8.394E-08 4.688E-07	3.019E-06 2.177E-09	3.540E-03 3.030E+02	4.731E-04 1.000E+03	3.609E-08	5.442E-07
5. 2.	1.483E-01 7.787E-07	4.000E-02 2.002E-15	1.813E-08 5.076E-02	7.203E-02 9.999E+02	5.216E-07 1.890E-06	2.365E-05 4.475E-09	1.052E-02 3.030E+02	5.523E-04 1.000E+03	7.441E-08	2.302E-06
4. 4.	1.569E-01 2.409E-05	1.372E-02 6.114E-15	2.076E-08 1.043E-01	2.182E-01 9.999E+02	4.784E-06 1.141E-05	2.296E-04 9.289E-09	2.701E-02 3.030E+02	4.421E-04 1.000E+03	1.547E-07	1.454E-05
4. 8.	1.301E-01 1.130E-03	3.832E-03 1.552E-14	2.012E-08 2.000E-01	5.644E-01 9.997E+02	3.606E-05 7.164E-05	1.444E-03 1.644E-08	5.958E-02 3.030E+02	3.165E-04 1.001E+03	2.771E-07	9.388E-05

E-5

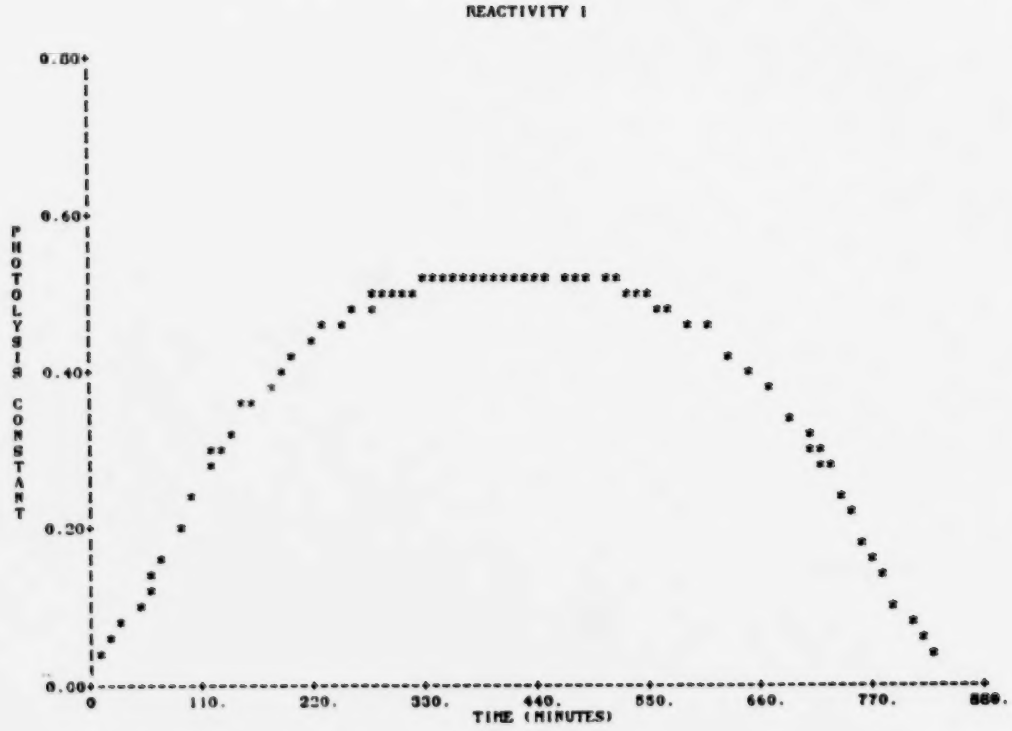
Output Results (Continued)

T LAT	E ANL	NO2 HOOH	NO O1D	O HCHO	O3 CH4	NO3 MEO2	N2O5 MEO	HNO3 TEMP	HONO M	OH	HO2
3.[illegible]E+02		9.397E-02	1.511E-03	1.029E-08	9.390E-01	1.111E-04	3.201E-03	9.311E-02	1.414E-04	2.262E-07	1.720E-04
6.[illegible]E+00		1.003E-02	2.403E-14	2.721E-01	9.993E+02	1.420E-04	1.277E-08	3.030E+02	1.001E+03		
6.[illegible]E+02		6.848E-02	7.973E-04	1.579E-08	1.150E+00	1.806E-04	3.972E-03	1.170E-01	6.566E-05	1.627E-07	1.860E-04
2.[illegible]E-01		2.456E-02	2.810E-14	2.909E-01	9.994E+02	1.813E-04	8.610E-09	3.030E+02	1.001E+03		
5.600E+02		5.027E-02	4.388E-04	1.244E-08	1.261E+00	2.730E-04	4.216E-03	1.346E-01	3.380E-05	1.123E-07	1.695E-04
2.[illegible]E-01		3.835E-02	2.603E-14	2.851E-01	9.993E+02	2.099E-04	5.490E-09	3.030E+02	1.001E+03		
7.200E+02		3.567E-02	2.101E-04	8.436E-09	1.295E+00	4.007E-04	4.472E-03	1.487E-01	1.729E-05	6.850E-08	1.310E-04
1.[illegible]E+00		4.800E-02	1.983E-14	2.709E-01	9.992E+02	2.307E-04	2.998E-09	3.030E+02	1.001E+03		
7.[illegible]E+02		1.801E-02	3.390E-03	3.242E-09	1.286E+00	1.110E-03	6.174E-03	1.624E-01	7.622E-06	2.286E-08	8.558E-05
1.[illegible]E+00		5.173E-02	8.839E-15	2.567E-01	9.992E+02	3.360E-04	6.821E-10	3.030E+02	1.001E+03		
8.[illegible]E+02		2.162E-03	1.676E-07	3.376E-10	1.270E+00	6.347E-03	4.219E-03	1.769E-01	4.079E-06	1.976E-09	3.731E-06
9.[illegible]E-01		5.191E-02	1.139E-15	2.409E-01	9.992E+02	6.961E-04	6.999E-12	3.030E+02	1.001E+03		

Output Results (Continued)



Output Results (Continued)



Output Results (Concluded)